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Volume I - Petroleum and Shale Oil Products

by

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Primarily, this effort has consisted of assembling data and has not included evaluation of data quality or the development of conclusions as to similarities and differences between a synfuel and its analogous petroleum product. Limitations of the data base are noted.

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ABSTRACT

This compendium of reported physical and chemical characterization data for petroleum and synthetic fuel products consolidates a large quantity of diverse data which have been generated and reported by numerous investigators over the past several decades. The products for which data have been compiled are: crude petroleum; raw and hydrotreated shale oil; raw and hydrotreated whole coal liquids and intermediates; and petroleum-, coal-, and shale-derived naphtha, jet and diesel fuels and other light fuel oils, heavy fuel oils, and residua. Coal liquids addressed are those from H-Coal, EDS, SRC-I and SRC-II direct coal liquefaction processes. Sixty-six individual properties relating to the following six characterization categories are covered: general physical and chemical properties; elemental composition data; hydrocarbon compound class properties; nitrogen-, oxygen-, and sulfur-containing compounds/compound class properties; properties of various distillation fractions; and properties of "non-primary" products and their distillation fractions.

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Much of the data contained in this compendium has been derived from documents and information provided to the authors by individuals/organizations engaged in synfuel development, petroleum and synfuel product characterization, and from related studies. The individuals and organizations who contributed to the data base compilation effort, and to whom the project is deeply indebted, are too numerous for complete listing in this report. The table which follows provides a listing of those individuals and organizations which provided substantial amounts of published and unpublished data in the form of copies of draft and final reports and journal articles for use in the preparation of the compendium.

The preparation of the draft of this compendium was carried out by TRW Energy and Environmental Division (the environmental element of which has since been acquired by Radian Corporation of Austin, TX), under EPA Contract No. 68-02-3174, Work Assignment Nos. 92 and 99. The revisions to the draft document and preparation of this final compendium were carried out by Multidisciplinary Energy and Environmental Systems and Applications (MEESA), Torrance, CA, under Purchase Order No. 19870 with Radian Corporation. The preparation of both draft and final documents has been under the technical direction of Dr. Masood Ghassemi, currently Principal and Technical Director of MEESA.

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1.0 BACKGROUND, OBJECTIVES, SCOPE AND OVERVIEW OF THE CURRENT DATA BASE

Under the Toxic Substances Control Act (TSCA), certain synthetic fuel products may be considered new chemical substances and, therefore, potentially subject to Premanufacture Notice (PMN) requirements which would require manufacturers to notify the U.S. Environmental Protection Agency (EPA) at least 90 days before they produce such substances for commercial purposes. Once notified, EPA has 90 days, extendable for good cause to 180 days, to review the chemical. During the review period, the Agency can act to prohibit or limit the manufacture, processing, or use of a new chemical substance when it makes certain findings.

Recognizing the possibility that certain synfuel products may be subject to TSCA's PMN requirements, a number of synfuel developers have held informal meetings with EPA to discuss related matters. As a first step toward developing the technical data base for use by EPA in comparing synfuel and petroleum products and providing guidance to synfuel developers on any PMN data submissions required for synfuel products, a data compilation effort has been undertaken through a contractual arrangement for the EPA's Office of Pesticides and Toxic Substances (OPTS). This data compilation effort, the result of which is this compendium, has involved collection and tabulation of the reported characterization data on major petroleum and shale- and coal-derived liquid fuels. Specific products addressed are: crude petroleum; raw and hydrotreated shale oil; raw and hydrotreated whole coal liquids and intermediates; and petroleum-, coal-, and shale-derived naphtha, jet and diesel fuels and other light fuel oils, heavy fuel oil, and residua. The coal liquids data cover only products from direct liquefaction of coal via H-Coal, EDS, SRC-I, and SRC-II processes.

The data presented in this compendium primarily consists of the characterization data which have been reported in the U.S. in the past several decades. Data for products from foreign sources and some older data (e.g., the older U.S. Bureau of Mines research on shale oil and coal liquids) are not included. There has been no attempt to evaluate the quality of the reported data, especially from the standpoint of analytical techniques and data reduction methods used. For this reason, it is recommended that the original reference be consulted to assure data suitability for specific use. In this document the units of measurement and the expression of various properties are those reported in the source documents; therefore, there are variations in the units of measurement and in some cases there are separate tabulations of parameters which are expressions of the same property (e.g., density, specific gravity, and API gravity)

Based on the data presented in this compendium and the discussions which have been held with scientists and other technical staff in various agencies and organizations supplying data for use in this project, the following are some general observations on the nature and limitations of the available data base on the physical and chemical characteristics of synfuel and petrofuel products.

- The data base on petroleum, shale oil, and coal liquid products is very diverse and the data have been generated by numerous investigators over the past several decades using a range of analytical procedures and test samples from a variety of origins including different raw material sources (e.g., coal types), processing scales (e.g., bench-/pilot-scale vs. commerical refineries), and operating conditions.

- Much of the reported characterization data do not include information on the detailed analytical methodology, source of sample (e.g., coal type), or operating conditions under which a refined product was obtained.

- In comparison with the relatively large volume of characterization data reported for coal liquids and shale oil products, surprisingly little data have been reported on the characteristics of the analogous petroleum products which have been in widespread use for many years. This is particularly true with respect to detailed compound characterization and individual compound identification. Thus, while considerable data are available on certain polynuclear aromatic hydrocarbons in coal liquids, analogous data are unavailable for petroleum counterparts.

- For all three product types (i.e., petroleum, shale oil, and coal liquids), the available detailed compositional data primarily relate to lighter "cuts". Detailed compositional analyses of petroleum and synfuel heavier cuts have not generally been carried out because of the very complex nature of these products which require a substantial amount of analytical effort. Such a costly effort, involving compound-by-compound identification, has not generally been considered justified because of the highly variable nature of the products and the questionable utility of the results since properties of the individual compounds may not be directly additive due to chemical interactions (e.g., associations, dimerizations, complex formation, etc.).

- Nearly all data on coal and shale oil products are from bench- and pilot-scale retorting/liquefaction units operated under a range of conditions aimed at establishing optimum conditions and developing design criteria for commercial scale plants. The products from these operations, for which characterization data have been reported, thus do not necessarily represent products expected from future commercial size units. This is particularly true for data from certain early pilot plant runs where extensive design/equipment changes have been made to the pilot plant operations thus making data from earlier runs obsolete or irrelevant.

- A considerable amount of the reported characterization data for refined shale oil products is for products obtained from the refining of 100,000 barrels of Paraho shale oil at Sohio's Toledo (Ohio) refinery.

- The characterization and compound type analyses of petroleum products have been conducted primarily for the purpose of improving processing conditions, refinery trouble shooting, enhancing product stability, and understanding better the geochemical phenomena of petroleum origins and formation processes. Similarly, the primary reason for oil shale and coal liquid characterization by compound class has been to identify better processing conditions from the standpoint of cost reduction.

- Some oil companies and synfuel developers appear to have some in-house characterization data on petroleum and synthetic fuel products. Such data are generally considered company proprietary and hence were not available for inclusion in this compendium.

2.0 DATA SOURCES AND ORGANIZATION OF THE COMPENDIUM

The major sources of data used in developing this compendium on physical and chemical characteristics of shale oil and petroleum products consisted of the extraction of data from published literature; telephone discussions and/or face-to-face interviews with research scientists and engineers at Department of Energy (DOE) National Laboratories and Energy Technology Centers; and data previously provided to TRW by major synfuel developers and potential synfuel users in connection with the preparation of the following three documents for EPA:

- "Environmental Aspects of Synfuel Utilization, EPA-600/7-81-025, March 1981.
- "Environmental Issues in Synfuel Development and End Use: The perspectives of Developers and Major Users", Draft Final Report submitted to EPA/IERL-RTP by TRW under Contract No. 68-02-3174, Work Assignment No. 60.
- "A Compendium of Synfuel End-Use Testing Programs", EPA-600/7-82-035, April 1982.

This compendium is organized into two volumes: Volume I, Petroleum and Shale Oil Products, and Volume II, Direct Coal Liquefaction Products. The reported data on product properties are presented in 356 tables which comprise this compendium. A list of these tables by title and page number and six indexes which identify the categories of products and properties covered by table number follow. The list of tables and the indexes are intended to serve as a directory to the material arrangement in the compendium.

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Index 1. General Physical and Chemical Properties by Table Numbers

Product	Specific Gravity	API Gravity	Viscosity	Pour Point	Carbon Residue	Density	Reid Vapor Pressure	Distillation Data	GC-Simulated Distillation	Refractive Index
Petroleum (Volume I)										
Crude	1	2	3	4	5	6	7	8	9	10
Naphtha	54	55	-*	-	-	56	57	58	59	60
Jet Fuel	73	74	75	76	-	77	78	79	80	81
Diesel Fuel	109	110	111	112	113	114	115	116	117	118
Residual Fuel	140	141	142	143	144	145	146	147	148	-
Shale Oil (Volume I)										
Raw	1	2	3	4	5	6	7	8	9	10
Naphtha	54	55	-	-	-	56	57	58	59	60
Jet Fuel	73	74	75	76	-	77	78	79	80	81
Diesel Fuel	109	110	111	112	113	114	115	116	117	118
Residual Fuel	140	141	142	143	144	145	146	147	148	-
Coal Liquids (Volume 2)										
Whole Process Liquids	163	164	170	171	172	165	-	166	167	168
Intermediates	194	195	199	200	201	196	-	197	198	-
Naphtha	224	225	233	234	235	226	227	228	229	-
Middle Distillate†	266	267	276	277	278	268	269	270	271	-
Heavy Distillate‡	308	309	318	319	320	310	311	312	313	272 314

(Continued)

Index 1. (Continued)

Product	Molecular Weight	Salt Content	Bottom Sediment and Water	Acidity	Gum Content	Flash Point	Freeze Point	Aniline Point/ Gravity	Water Tolerance/ Separometer Index	Smoke Point
Petroleum (Volume I)										
Crude	11	12	13	14	-	-	-	-	-	-
Naphtha	61	-	-	62	63	-	-	-	-	-
Jet Fuel	82	-	83	84	92	85	86	87,88	89,90	91
Diesel Fuel	119	-	120	121	-	122	-	124	-	-
Residual Fuel	-	-	149	150	-	151	-	-	-	-
Shale Oil (Volume I)										
Crude	11	12	13	14	-	-	-	-	-	-
Naphtha	61	-	-	62	63	-	-	-	-	-
Jet Fuel	82	-	83	84	92	85	86	87,88	89,90	91
Diesel Fuel	119	-	120	121	-	122	-	124	-	-
Residual Fuel	-	-	149	150	-	151	-	-	-	-
Coal Liquids (Volume 2)										
Whole Process Liquids	169	-	-	-	-	-	-	174	-	-
Intermediates	-	-	-	-	-	202	-	-	-	-
Naphtha	230	-	236	231	232	238	237	241	-	239
Middle Distillate†	273	-	279	274	275	281	280	284	-	282
Heavy Distillate‡	315	-	321	316	317	323	322	-	-	-

(Continued)

Index 1 (Continued)

Product	Heat of Combustion	Thermal Stability	Corrosion Rating	WSIM	Anti-Icing	Cloud Point	Cetane Index	Bromine Number	Heat Capacity
Petroleum (Volume I)									
Crude	-	-	-	-	-	-	-	-	-
Naphtha	-	-	-	-	-	-	-	-	-
Jet Fuel	93	94	95	96	97	-	-	-	-
Diesel Fuel	125	-	126	-	-	123	127	-	-
Residual Fuel	-	-	-	-	-	-	-	-	-
Shale Oil (Volume I)									
Crude	-	-	-	-	-	-	-	-	-
Naphtha	-	-	-	-	-	-	-	-	-
Jet Fuel	93	94	95	96	97	-	-	-	-
Diesel Fuel	125	-	126	-	-	123	127	-	-
Residual Fuel	-	-	-	-	-	-	-	-	-
Coal Liquids (Volume 2)									
Whole Process Liquids	173	-	-	-	-	-	-	175	-
Intermediates	203	-	-	-	-	-	-	205	204
Naphtha	240	-	243	-	-	-	-	242	-
Middle Distillate[†]	283	-	286	-	-	-	-	285	-
Heavy Distillate[‡]	324	-	326	-	-	-	-	325	332

(Continued)

Index 1. (Concluded)

Product	Color	Research Octane Number	Moisture	Sintering Temperature	Melting (Fusion) Point	Softening Point	Free Swelling Index	Ash (Proximate)	Volatiles Content	Fixed Carbon
Petroleum (Volume I)										
Crude	-	-	-	-	-	-	-	-	-	-
Naphtha	-	-	-	-	-	-	-	-	-	-
Jet Fuel	-	-	-	-	-	-	-	-	-	-
Diesel Fuel	-	-	-	-	-	-	-	-	-	-
Residual Fuel	-	-	-	-	-	-	-	-	-	-
Shale Oil (Volume I)										
Crude	-	-	-	-	-	-	-	-	-	-
Naphtha	-	-	-	-	-	-	-	-	-	-
Jet Fuel	-	-	-	-	-	-	-	-	-	-
Diesel Fuel	-	-	-	-	-	-	-	-	-	-
Residual Fuel	-	-	-	-	-	-	-	-	-	-
Coal Liquids (Volume 2)										
Whole Process Liquids	-	-	-	-	-	-	-	-	-	-
Intermediates	206	-	-	-	-	-	-	-	-	-
Naphtha	245	246	244	-	-	-	-	-	-	-
Middle Distillate†	288	-	287	-	-	-	-	-	-	-
Heavy Distillate‡	-	-	327	328	329	330	331	333	334	335

Explanatory Notes

*Dash indicates no table was prepared for the subject category due to lack of available data or irrelevance of the subject category to a particular product

†Includes jet and diesel fuels and other light fuel oils

‡Includes heavy fuel oils

Index 2. Elemental Composition Data by Table Number

Product	Oxygen Content	Sulfur Content	Nitrogen Content	Carbon Content	Hydrogen Content	H/C Weight Ratio	Trace Element Content	Ash Content (Ultimate Analysis)
Petroleum (Volume I)								
Crude	15	16	17	18	19	20	21	-*
Naphtha	64	65	66	67	68	-	69	-
Jet Fuel	98	99	100	101	102	-	103	-
Diesel Fuel	128	129	130	131	132	-	133	134
Residual Fuel	152	153	154	155	156	-	157	-
Shale Oil (Volume I)								
Crude	15	16	17	18	19	20	21	-
Naphtha	64	65	66	67	68	-	69	-
Jet Fuel	98	99	100	101	102	-	103	-
Diesel Fuel	128	129	130	131	132	-	133	134
Residual Fuel	152	153	154	155	156	-	-	157
Coal Liquids (Volume 2)								
Whole Process Liquids	176	177	178	179	180	-	181	182
Intermediates	207	208	209	210	211	-	212	213
Naphtha	247	248	249	250	251	-	252	-
Middle Distillate†	289	290	291	292	293	-	294	295
Heavy Distillate‡	336	337	338	339	340	-	341	342

Explanatory Notes

*Dash indicates no table was prepared for the subject category due to lack of available data or irrelevance of the subject category to a particular product

†Includes jet and diesel fuels and other light fuel oils

‡Includes heavy fuel oils

Index 3. Hydrocarbon Compound Class Properties by Table Number

Product	Saturates	Olefins	Aromatics	Individual Hydrocarbon/ Hydrocarbon Classes (Including PNA's)	Hydrocarbon Compound Classes by Solvent Fractionation	Elemental Composition for Hydrocarbon Classes by Solvent Fractionation
Petroleum (Volume I)						
Crude	22,25,28,31	23,26,29,32	24,27,30,33	36,37	34,35	-*
Naphtha	70	70	70	71	-	-
Jet Fuel	104	104	104	105	-	-
Diesel Fuel	135	135	135	136,137	-	-
Residual Fuel	158	158	158	159,160	-	-
Shale Oil (Volume I)						
Crude	22,25,28,31	23,26,29,32	24,27,30,33	36,37	34,35	-
Naphtha	70	70	70	71	-	-
Jet Fuel	104	104	104	105	-	-
Diesel Fuel	135	135	135	136,137	-	-
Residual Fuel	158	158	158	159,160	-	-
Coal Liquids (Volume 2)						
Whole Process Liquids	183	-	183	184	185	-
Intermediates	214	214	214	215	216	-
Naphtha	253	253	253	254	-	-
Middle Distillate†	296	296	296	297	-	-
Heavy Distillate‡	343	343	343	344,345	346	347

Explanatory Notes

*Dash indicates no table was prepared for the subject category due to lack of available data or irrelevance of the subject category to a particular product

†Includes jet and diesel fuels and other light fuel oils

‡Includes heavy fuel oils

Index 4. Nitrogen-, Oxygen-, and Sulfur-Containing Compounds/Compound Class Properties by Table Number

Product	Nitrogen-Containing Compounds	Sulfur-Containing Compounds	Oxygen-Containing Compounds	Nitrogen/Oxygen/Sulfur Compound Classes by Solvent Fractionation
Petroleum (Volume I)				
Crude	38,39,40	45,46	45,46	41,42,43,44
Naphtha	-*	-	-	72
Jet Fuel	-	108	-	106,107
Diesel Fuel	-	-	-	138,139
Residual Fuel	162	-	-	161
Shale Oil (Volume I)				
Crude	38,39,40	45,46	45,46	41,42,43,44
Naphtha	-	-	-	72
Jet Fuel	-	108	-	106,107
Diesel Fuel	-	-	-	138,139
Residual Fuel	-	-	-	161
Coal Liquids (Volume 2)				
Whole Process Liquids	186	187	-	-
Intermediates	217	217	217	218,219
Naphtha	255	255	255	-
Middle Distillate†	298	298	298	299
Heavy Distillate‡	348,349	348,349	348	350

Explanatory Notes

*Dash indicates no table was prepared for the subject category due to lack of available data or irrelevance of the subject category to a particular product

†Includes jet and diesel fuels and other light fuel oils

‡Includes heavy fuel oils

Index 5. Properties of Various Distillation Fractions by Table Number

Product	General Physical/ Chemical Properties	Elemental Composition	Hydrocarbon Compound Classes	Nitrogen-, Oxygen-, & Sulfur-Containing Compounds
Petroleum (Volume I)				
Crude	47,48	47,48	53	51,52,53
Naphtha	-	-	-	-
Jet Fuel	-	-	-	-
Diesel Fuel	-	-	-	-
Residual Fuel	-	-	-	-
Shale Oil (Volume I)				
Crude	49,50	49,50	49,50	49,50
Naphtha	-	-	-	-
Jet Fuel	-	-	-	-
Diesel Fuel	-	-	-	-
Residual Fuel	-	-	-	-
Coal Liquids (Volume 2)				
Whole Process Liquids	188	189	190,191,192,193	-
Intermediates	220	221	222	222,223
Naphtha	256	257	258	258
Middle Distillate[†]	300	301	-	-
Heavy Distillate[‡]	351	352	353	-

Explanatory Notes

*Dash indicates no table was prepared for the subject category due to lack of available data or irrelevance of the subject category to a particular product

[†] Includes jet and diesel fuels and other light fuel oils

[‡] Includes heavy fuel oils

Index 6. Properties of Non-Primary Products[*] and Distillation Fractions by Table Number

Product	General Physical/ Chemical Properties	Elemental Composition	Hydrocarbon Compound Classes	Nitrogen-, Oxygen-, & Sulfur-Containing Compounds
Petroleum (Volume I)				
Naphtha	-[†]	-	-	-
Jet Fuel	-	-	-	-
Diesel Fuel	-	-	-	-
Residual Fuel	-	-	-	-
Shale Oil (Volume I)				
Naphtha	-	-	-	-
Jet Fuel	-	-	-	-
Diesel Fuel	-	-	-	-
Residual Fuel	-	-	-	-
Coal Liquids (Volume 2)				
Naphtha				
-whole	259,260	261	262	-
-distillation fractions	263	264	265	-
Middle Distillate[‡]				
-whole	302	304	306	-
-distillation fractions	303	305	307	-
Heavy Distillate[§]	354	355	356	-

Explanatory Notes

[*] As used in this compendium, non-primary products refer to materials obtained from heavier cuts or intermediates (e.g., via distillation).

[†] Dash indicates no table was prepared for the subject category due to lack of available data or irrelevance of the subject category to a particular product.

[‡] Includes jet and diesel fuels and other light fuel oils.

[§] Includes heavy fuel oils.

3.0 GLOSSARY

3.1 SAMPLE SOURCES/DESCRIPTIONS

API RO-1, RO-2, RO-3, RO-4 -- Crude shale oils used in a blind American Petroleum Institute characterization test program, and derived from the Union B, Paraho direct, Paraho indirect, or Colony Semi-works retorts.

Dearsenited shale oil -- The material resulting from the processing of raw shale oil in two dearseniting reactors operating in series at elevated temperatures and pressures, which remove arsenic and hydrogen unsaturated hydrocarbons from raw shale oil and thus stabilize it for further processing. This treatment is also called "mild" or "1st-stage" hydrotreatment.

Dewaxed syncrude -- The material resulting from the processing of the dearsenited shale oil in a second stage hydrotreating unit for the removal of nitrogen and sulfur, followed by processing in a dewaxing reactor and a final stripper for the removal of light ends.

EDS development unit -- 75-lb/day development unit, also referred to as the recycle coal liquefaction unit (RCLU); located in Baytown, TX, and operated since 1964.

EDS pilot plant -- One-tpd coal liquefaction pilot plant (CLPP); located in Baytown, TX, and operated since the mid-1970s. CLPP is normally operated in the "once-through mode" which involves no recycling of vacuum bottoms and operation at moderate temperatures (800°F). CLPP can also be operated in a "vacuum gas oil mode" which operates at higher temperatures (800-1000°F) and has a high yield of vacuum gas oil.

Ft. Lewis pilot plant -- 50-tpd pilot plant for the SRC-I and SRC-II processes; located in Ft. Lewis, Washington, and operated since the early 1970s.

Geokinetics - HRI -- Refining effort conducted in 1980 at Hydrocarbon Research, Inc., Lawrenceville, NJ, process development unit on raw shale oil produced by Geokinetics, Inc., at Anvil Points, CO.

H-Coal bench-scale unit -- Small bench-scale unit located in Lawrenceville, NJ, and operating since the early 1960s. The unit can be operated in both "Syncrude mode" and "fuel oil mode". The syncrude mode utilizes higher temperatures and pressures and more hydrogen for liquefaction than the fuel oil mode, and produces a lower yield of residual fuel oil but higher yields of other syncrudes. The fuel oil mode produces low sulfur fuel oil as the major product; this mode utilizes lower temperatures and pressures and less hydrogen for liquefaction than the syncrude mode, and requires a separate liquid-solid separation unit.

H-Coal PDU -- 3-tpd PDU located in Lawrenceville, NJ, and operating since 1975. Like the H-Coal bench-scale unit, this unit can be operated in both the syncrude and fuel oil modes.

IGT Hytort -- Institute of Gas Technology's Hytort process development unit in Chicago, IL.

In-Situ; Rock Springs, WY -- Laramie Energy Technology Center/Department of Energy in-situ retort at Rock Springs, WY; the oil shale at the site is part of the Green River oil shale formation.

In-Situ; Rock Springs, WY - LETC -- Refining effort conducted by the Laramie Energy Technology Center on raw shale oil from the LETC in-situ retort at Rock Springs, WY.

Occidental modified in-situ -- Occidental Petroleum Co. retort at Logan Wash, CO. The modified in-situ process involves the retorting of a rubblized column of broken shale formed by expansion of the oil shale into a previously mined out void volume.

Occidental modified in-situ, LETC -- Refining effort conducted by the Laramie Energy Technology Center in the late 1970s on raw shale oil from the Occidental Petroleum Co. modified in-situ retort at Logan Wash, CO (see above).

Paraho-Chevron -- Refining effort conducted by the Chevron Research Company, Salt Lake City, Utah, in 1978 on raw shale oil produced by the Paraho direct heat retort process.

Paraho-SOHIO, Gary Western -- Refining effort conducted in 1976 at Standard Oil of Ohio's Gary Western refinery on 10,000 bbl of raw shale oil produced at Anvil Points, CO, by the Paraho direct heat retort process, under DOD's synthetic fuel development program.

Paraho-SOHIO, Toledo -- Refining effort conducted in late 1978 at Standard Oil of Ohio's Toledo refinery on 100,000 bbl of raw shale oil produced at Anvil Points, CO, by the Paraho direct heat retort process, under DOD's synthetic fuel development program.

TOSCO-II, ARCO and ARCO-1 -- Refining effort conducted by the Atlantic Richfield Co. in 1977 on raw shale oil produced by the Oil Shale Corporation using the TOSCO-II process at Parachute Creek, CO.

Wilsonville pilot plant -- 6-tpd pilot plant for the SRC-II process; located in Wilsonville, AL, and operating since the mid 1960s.

3.2 ABBREVIATIONS AND SYMBOLS

EDS - Exxon Donor Sovent

H-Coal - A liquefaction process developed by Hydrocarbon Research

NA - Data are not available

ND - None detected; substance of interest was not detected

PDU - Process development unit

SRC - Solvent Refined Coal

Z Number - Term used to designate the number of rings plus double bonds in a chemical compound identified by mass spectrometry

"--" - Indicates "not applicable" or "not relevant"

Part I. Petroleum Crude, Raw Shale Oil and Hydrotreated Shale Oil

Table 1. Specific Gravity

Material	Value	Sample Description/Source	Reference
Petroleum crude	0.729 to 1.008	Range for 800 U. S. crudes	3
Raw shale oil	0.9315, 0.9383 (60°F)	Paraho	33,38
	0.8800	In-situ; Rock Springs, WY	44,46
Hydrotreated shale oil	0.8086 (60/60°F)	In-situ; Rock Springs, WY	44,46
	0.833 (60/60°F)	TOSCO II, Arco	50

Table 2. API Gravity

Material	Value (degrees)	Sample Description/Source	Reference
Petroleum crude	8.9 to 62.6	Range for 800 U. S. crudes	3
Raw shale oil	19.3, 20.2, 20.4	Paraho	33,38-39
	19.3, 20.7, 20.7	TOSCO II	40
	25.0	Modified in-situ, Occidental	39
Hydrotreated shale oil	33.8	Paraho-SOHIO Toledo	37
	43.6	In-situ; Rock Springs, WY	44,46
	38.4	TOSCO II, Arco	50

Table 3. Viscosity (Saybolt Universal at 100°F)

Material	Value (seconds)	Sample Description/Source	Reference
Petroleum crude	28 to 7,648	Range for 794 U. S. crudes	3
Raw shale oil	213	Paraho	37
	96	TOSCO II	41
	45, 78	In-situ; Rock Springs, WY	46,45
	107.2, 125.7, 131.6, 174.2	4 API retort oils	40
Hydrotreated shale oil	46	Paraho-SOHIO Toledo	37
	45	In-situ; Rock Springs, WY	44,46
	38	TOSCO II, Arco	50

Table 4. Pour Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum crude	<5 to 125	Range for 800 U. S. crudes	3
Raw shale oil	85	4 Paraho samples	33,35,37,38
	90	Paraho	39
	75, 80, 50, 80	3 samples of TOSCO and one sample of TOSCO II, respectively	40,41
	-10, 40, 40	In-situ; Rock Springs, WY	35,45,46
	25	Modified in-situ, Occidental	39
	65, 70, 80, 85	4 API retort oils	40
	64	NA	57
Hydrotreated shale oil	85	2 samples of Paraho-SOHIO Toledo	35,37
	75	Mildly hydrotreated shale oil	57
	45	Dewaxed syncrude	57

Table 5. Carbon Residue

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum crude	Nil (<0.009) to 14.0*	Range for 800 U. S. crudes	3
Raw shale oil	1.383, 1.85 and 2.977[†]	Paraho	38,39,33
	0.54[†]	Modified in-situ, Occidental	39
Hydrotreated shale oil	NA	--	--

Explanatory Notes

*Conradson carbon residue
[†] Ramsbottom carbon

Table 6. Density

Material	Value (g/ml)	Sample Description/Source	Reference
Petroleum crude	0.9472	E. Wilmington crude	57
	0.9931	San Joaquin Valley crude	57
Raw shale oil	0.9290 (60°F)	Paraho	35
	0.9116 (60°F)	In-situ; Rock Springs, WY	35
	0.9277, 0.9254, 0.9323, 0.9393	4 API retort oils	40
	0.9273	NA	57
Hydrotreated shale oil	0.8610 (60°F)	Paraho-SOHIO Toledo	35
	0.9042	Mildly hydrotreated shale oil	57
	0.8388	Dewaxed syncrude	57

Table 7. Reid Vapor Pressure

Material	Value (psi)	Sample Description/Source	Reference
Petroleum crude	1.6	E. Wilmington crude	57
Raw shale oil	0.7	NA	57
Hydrotreated shale oil	0.4	Mildly hydrotreated shale oil	57
	0.7	Dewaxed syncrude	57

Table 8. Distillation Data

Material	Value (%)	Sample Description/Source	Reference
Petroleum crude*	--	--	--
Raw shale oil	IBP/400°F - 5	Paraho	37
	400/650°F - 28		
	650/900°F - 62		
	IBP/400°F - 6.07, 7.20, 9.91, 17.30	4 API retort oils	40
	400/650°F - 25.87, 25.96 27.99, 30.17		
	650/850°F - 19.43, 25.33, 28.92, 34.31		
	850+°F - 27.66, 34.63 35.87, 39.66		
Hydrotreated shale oil	400°F - 13	Paraho-SOHIO Toledo	37
	650°F - 52		
	900°F - 90		

Explanatory Notes

*Extensive distillation data are available for 800 U. S. petroleum crudes, using Bu Mines distillation method, involving distillation at 760 mm Hg and taking cuts from IBP to 122°F, up to 527°F in 45°F temperature intervals, followed by distillation at 40 mm Hg from 392°F to 572°F in 45° temperature intervals, and collection of residue above 572°F.

Table 9. GC Simulated Distillation Data*

Material	Boiling Point Range, °C	Sample Description/Source	Reference
Petroleum crude	5% recovered - 124 50% recovered - 368 90% recovered - NA 95% recovered - NA 87.1% recovered - 535	E. Wilmington crude	57
	5% recovered - 200 50% recovered - 339 90% recovered - 481 95% recovered - 515 97.6% recovered - 535	San Joaquin Valley crude	57
Raw shale oil	5% recovered - 196 50% recovered - 381 90% recovered - 523 92.0% recovered - 535	Paraho	57
	5% recovered - 166 50% recovered - 268 90% recovered - 411 99.1% recovered - 535	In-situ; Rock Springs, WY	57
	5% recovered - 163 50% recovered - 379 90% recovered - 518 92.9% recovered - 535	NA	57

(Continued)

Table 9 (Concluded)

Material	Boiling Point Range, °C	Sample Description/Source	Reference
Hydrotreated shale oil	5% recovered - 151 50% recovered - 333 90% recovered - 468 95% recovered - 506 97.2% recovered - 535	Paraho-SOHIO Toledo	57
	5% recovered - 154 50% recovered - 377 90% recovered - 513 95% recovered - NA 94.0% recovered - 535	Mildly hydrotreated shale oil	57
	5% recovered - 135 50% recovered - 304 90% recovered - 455 95% recovered - 490 98.8% recovered - 535	Dewaxed syncrude	57

Explanatory Notes

*GC simulated distillation involves use of gas chromatograph rather than distillation column. Retention times of sample peaks are based on retention times of a calibration mixture of C_3 to C_{42} normal paraffins. The boiling range distribution of the sample is calculated in weight percent via computer. Volume percent values are calculated from a density - boiling point correlation of normal paraffins (Reference 35).

Table 10. Refractive Index

Material	Value (Abbe refractometer, 67°C)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	--*	One Paraho and one in-situ; Rock Springs, WY sample	35
Hydrotreated shale oil	1.46	Paraho-SOHIO Toledo	35

Explanatory Notes

*Samples too dark for analysis.

Table 11. Molecular Weight (Cryoscopic)

Material	Value	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	310, 326	2 Paraho samples	35,39
	234	In-situ; Rock Springs, WY	35
	279	Modified in-situ, Occidental	39
	230, 265, 272, 274	4 API retort oils	40
Hydrotreated shale oil	245	Paraho-SOHIO Toledo	35

Table 11. Molecular Weight (Cryoscopic)

Material	Value	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	310, 326	2 Paraho samples	35,39
	234	In-situ; Rock Springs, WY	35
	279	Modified in-situ, Occidental	39
	230, 265, 272, 274	4 API retort oils	40
Hydrotreated shale oil	245	Paraho-SOHIO Toledo	35

Table 12. Salt Content

Material	Value (lb/M* bbl)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	4.9 (8.2)†, unsettled	Paraho	33
Hydrotreated shale oil	NA	--	--

Explanatory Notes

*M = one thousand.

†Reference does not indicate whether values for raw shale oil refer to one or two shale samples.

Table 13. Bottom Sediment and Water

Material	Value (vol. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	0.1 and 0.1*	2 Paraho samples	35,39
	2.8*	In-situ; Rock Springs, WY	35
	0.0*	Modified in-situ, Occidental	39
Hydrotreated shale oil	0.2	Paraho-SOHIO Toledo	35

Explanatory Notes

*Determined via ASTM D-96.

Table 14. Total Acid Number

Material	Value (mg KOH/g)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	1.969, 1.988	2 Paraho samples	38,33
Hydrotreated shale oil	NA	--	--

Table 15. Oxygen Content

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum crude	0.0004	E. Wilmington crude	57
	0.61	San Joaquin Valley crude	57
Raw shale oil	1.05, 1.16, 1.38, 1.38, 1.40	Paraho	35,39,33,37,38
	0.6, 0.80	In-situ; Rock Springs, WY	43,57
	1.52	NA	57
Hydrotreated shale oil	0.026	Paraho-SOHIO, Toledo	57
	1.28	Mildly hydrotreated shale oil	57
	0.012	Dewaxed syncrude	57

Table 16. Sulfur Content

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum crude*	Nil (0.00) to 5.93	Range for 800 U. S. crudes	3
Raw shale oil	0.61,0.66,0.70,0.70,0.70	Paraho	38,39,33,35,37
	0.72,0.82,0.82,0.95,1.1	In-situ; Rock Springs, WY	43-46,57
	0.8	NA	57
Hydrotreated shale oil	0.0003	Paraho-SOHIO, Toledo	57
	0.37	Mildly hydrotreated shale oil	57
	0.0014	Dewaxed syncrude	57

Explanatory Notes

*Low sulfur crudes are those having sulfur contents in the range of 0 to <0.5%; high sulfur crudes are those having sulfur contents in the range of >1.35% (Reference 7).

Table 17. Nitrogen Content

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum crude	0.0000 to 0.936	Range for 685 U. S. crudes	1,3
Raw shale oil	2.02,2.02,2.18,2.19,2.20	Paraho	33,37,39,38,35
	1.4,1.41,1.50,1.62,1.62	In-situ; Rock Springs, WY	43-46,57
	1.7	NA	57
Hydrotreated shale oil	0.33	Paraho-SOHIO, Toledo	57
	1.4	Mildly hydrotreated shale oil	57
	0.0052	Dewaxed syncrude	57

Table 18. Carbon Content

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum crude	NA*	--	--
Raw shale oil	83.68,84.30,84.9,84.9	Paraho	33,39,38,35
	84.0,84.1,84.5,84.7	TOSCO II	40
	84.57,85.45,85.46	IGT Hytort	42
	84.61,85.0	In-situ; Rock Springs, WY	43,44
	85.78	Modified in-situ, Occidental	39
Hydrotreated shale oil	86.6	Paraho-SOHIO Toledo	35
	87.30,88.27	IGT Hytort	42

Explanatory Notes

*Data currently being developed and computerized at DOE's Bartlesville Energy Technology Center, Bartlesville, OK.

Table 19. Hydrogen Content

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum crude	NA*	--	--
Raw shale oil	11.17,11.29,11.5,11.50	Paraho	33,35,39,38
	10.7,11.1,11.3,11.3	TOSCO II	40
	9.42,9.56,11.40	IGT Hytort	42
	12.0,12.08	In-situ; Rock Springs, WY	43,44
	12.08	Modified in-situ, Occidental	39
Hydrotreated shale oil	13.1	Paraho-SOHIO Toledo	35
	11.70,12.60	IGT Hytort	42

Explanatory Notes

*Data currently being developed and computerized at DOE's Bartlesville Energy Technology Center, Bartlesville, OK.

Table 20. H/C Weight Ratio

Material	Value	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	0.110,0.112,0.135	IGT Hytort	42
Hydrotreated shale oil	0.133,0.144	IGT Hytort	42

Table 21. Trace Elements (ppmw)*

Material	Al	Sb	As	Be	Cd	Ca	Cl	Cr	Co	Cu	Fe	Pb	Mg	Mn	Hg	Mo	Ni
Petroleum Crude	3.8	0.44	0.8	0.08	2.27	14	12	1.3	2.21	2.8	18	3.5	13	1.33	0.04	0.90	42.2
	NA	ND <0.3	0.5	NA	0.01	NA	NA	0.5	NA	0.06	34	0.2	NA	NA	ND <1	NA	58
	NA	ND <0.5	ND <0.3	NA	0.03	NA	NA	0.8	NA	0.3	47	0.3	NA	NA	ND <1	NA	63
Raw shale oil	1.5 (FE)	ND <3	7.5 to 29	ND <0.005	0.010	3.8 (FE)	ND <2	0.036 (FE)	1.0	0.035	53 to 70	0.06 (FE)	2.1 (AA)	0.092 (FE)	ND <2	0.07 (FE)	2 to 3.2
	NA	NA	8.0 to 32.0	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
	66 (FE)	11	5.4	<0.01	0.2	88 (FE)	67	0.5 (FE)	1.3	15	164	6.0 (FE)	46 (AA)	1.3 (FE)	4	1.6 (FE)	4.1 (FE)
	NA	NA	18	NA	NA	NA	NA	NA	NA	NA	27	NA	NA	NA	NA	NA	6.5
	NA	NA	33 to 55	NA	NA	NA	NA	NA	NA	NA	4.9 to 46	NA	NA	NA	NA	NA	1.3 to 2.4
	NA	0.5	34	NA	0.01	NA	NA	0.16	NA	0.36	9.1	0.2	NA	NA	ND <1	NA	1.6
Hydrotreated shale oil	0.040 (FE)	ND <3(FE)	<0.5 (XRF)	<0.005 (AA)	ND <0.005 (AA)	0.052 (FE)	ND <2 (FE)	0.010 (FE)	ND <0.03 (FE)	0.030 (AA)	0.24 (FE)	ND <0.06 (FE)	0.002 (AA)	<0.005 (FE)	ND <2 (XRF)	ND <0.02 (FE)	<0.05 (FE)
	NA	ND<0.5	1.0	NA	ND <0.03	NA	NA	0.34	NA	0.05	0.3	0.2	NA	NA	ND<1	NA	ND <0.05

(Continued)

Table 21 (Concluded)

Material	K	Se	Si	Ag	Na	Sr	Th	Sn	Ti	V	Zn	Sample Description/Source	Reference
Petroleum Crude	34	0.7	17.5	0.3	31	0.15	0.2	6.2	1.8	160	1.26	Average of several domestic and imported crudes	26
	NA	ND <0.3	NA	NA	NA	NA	NA	NA	NA	36	1.1	E. Wilmington crude	57
	NA	ND <0.3	NA	NA	NA	NA	NA	NA	NA	73	1.5	San Joaquin crude	57
Raw shale oil	0.17	ND <0.5 (XRD)	7.4 (AA)	ND (<0.01) (FE)	<0.3 to 1.1	0.034 (FE)	ND <6	<0.5 (AA)	<0.4	0.17 to 0.28 (FE)	1.7	Range of 4 Paraho samples	33 35 37 39
	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	Range of 3 TOSCO samples	40
	NA	0.8	202 (AA)	<0.03 (FE)	380	1.4 (FE)	ND <6	0.6 (AA)	9	0.5 (FE)	233	In-situ; Rock Springs, WY	35
	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	Modified in-situ, Occidental	39
	NA	NA	NA	NA	2.1 to 3.1	NA	NA	NA	NA	0.10 to 0.55	NA	Range of 4 API Retort oils	40
	NA	0.8	NA	NA	NA	NA	NA	NA	NA	1.0	1.7	NA	57
Hydrotreated shale oil	NA	ND <0.6 (XRF)	<0.3 (AA)	<0.01 (FE)	0.15 (FE)	0.003 (FE)	ND <6 (XRF)	<0.5 (AA)	ND <0.4 (XRF)	<0.03 (FE)	0.064 (AA)	Paraho - SOHIO Toledo	35
	NA	ND (<0.3)	NA	NA	NA	NA	NA	NA	NA	0.07	0.02	Dewaxed syncrude	57

Explatory Notes

*Methods used include atomic absorption spectrocopy (AA), flame emission spectroscopy (FE), neutron activation analysis (NAA) and X-ray fluoresence (XRF).

Table 22. Saturates (Paraffins + Naphthenes)* in Light Boiling Fractions (IBP to approximately 400°F)

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum crude	100.0, 97.7, 96.2, 94.6, 90.8†	Wilmington, CA crude	4
	100.0, 96.8, 95.9, 91.0, 83.6, 82.8, 81.8‡	Recluse, WY crude	4
	96.6, 88.7, 86.0, 80.4, 77.0, 75.0§	Prudhoe Bay, AK crude	5
	93.8, 87.4, 80.8, 80.4, 84.2#	Alaskan North Slope crude	6
	93**	API Crude Oil C	58
	91**	API Crude Oil D	58
Raw shale oil	35.2	Paraho - SOHIO Toledo	35
	48.2,65.2	In-situ; Rock Springs, WY	35,81
Hydrotreated shale oil	84.6	Paraho - SOHIO Toledo	35

Explanatory Notes

*Naphthene (i.e., cycloparaffin) compound types in the subject boiling range are generally one- and two-ring paraffins.

†Values are for 5 fractions corresponding to 45°F interval with cut points of 212, 257, 302, 347, and 392°F and accounting for 2.3, 2.4, 2.4, 2.5 and 2.8 Vol. % of crude, respectively.

**Values are for fractions boiling between 120°F and 350°F.

#Values are for the following 5 distillation fractions: 55-165°F, 165-220°F, 220-280°F, 380-340°F and 340-380°F.

‡Values for 7 distillation fractions beginning at 122°F and taken at 45°F intervals up to 392°F, and accounting for 3.7, 2.7, 6.1, 8.2, 6.3, 5.7 and 4.7 Vol. % of crude, respectively.

§Values are for 6 fractions corresponding to 45°F interval cut points of 167, 212, 257, 302, 347 and 392°F and accounting for 2.1, 2.6, 3.5, 3.6, 3.7 and 3.5 Vol. % of crude, respectively.

Table 23. Olefins in Light Boiling Fractions
(IBP to approximately 400°F)

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	36.7	Paraho - SOHIO Toledo	35
	10.2,11.1	In-situ; Rock Springs, WY	35,81
Hydrotreated shale oil	NA	--	--

Table 24. Aromatics in Light Boiling Fractions*
(IBP to approximately 400°F)

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum crude	0.0, .2.3, 3.7, 5.4, 9.2 †	Wilmington, CA crude	4
	3.2, 4.1, 9.0, 16.4, 17.2, 18.2‡	Recluse, WY crude	4
	3.4, 11.3, 14.0, 19.6, 23.0, 25.0§	Prudhoe Bay, AK crude	5
	6.24, 10.57, 19.21, 19.56, 15.84#	Alaskan North Slope crude	6
	7.4**	API Crude Oil C	58
	9.0**	API Crude Oil D	58
Raw shale oil††	21.2	Paraho - SOHIO Toledo	35
	23.9,23.7##	In-situ; Rock Springs, WY	35,81
Hydrotreated shale oil§§	15.4	Paraho - SOHIO Toledo	35

Explanatory Notes

*Aromatics in the subject boiling range consist of mono- and diaromatics (i.e., alkyl benzenes, naphthene benzenes and naphthalenes).

#Values are for the following 5 distillation fractions: 55-165°F, 165-220°F, 220-280°F. 280-340°F and 340-380°F.

††Values of 370 ppmw, 57 ppmw and 1600 ppmw are reported for Paraho, in-situ Rock Springs, WY, and a third raw shale oil, respectively (Reference 57).

##Values include sulfur, nitrogen and oxygen compounds.

§§Benzene values of 320 ppmw for a mildly hydrotreated shale oil and 40 ppmw for a dewaxed syncrude are reported in Reference 57; a value of 400 ppmw for Paraho - SOHIO Toledo hydrotreated shale oil is also reported (Reference 57).

†Values are for 5 fraction corresponding to 45°F interval cut points of 212, 257, 302, 347 and 392°F and accounting for 2.3, 2.4., 2.4, 2.5 and 2.8 Vol. % of crude, respectively.

‡Values are for 6 fractions corresponding to 45°F interval cut points of 167, 212, 257, 302, 347 and 392°F and accounting for 2.7, 6.1, 8.2, 6.3, 5.7 and 4.7 Vol. % of crude, respectively.

§Values are for 6 fractions corresponding to 45°F interval points of 167, 212, 257, 302, 347 and 392°F and accounting for 2.1, 2.6, 3.5, 3.6, 3.7 and 3.5 Vol. % of crude, respectively.

**Values are for fractions boiling between 120°F and 350°F.

Table 25. Saturates (Paraffins* + Naphthenes) in Medium Boiling Fractions (Approximately 400°F to 650°F)

Material	Value (V = Vol. %; W = Wt. %)	Sample Description/Source	Reference
Petroleum crude	77.6, 77.8, 78.4, 76.2, 69.7† V	Wilmington, CA crude	4
	80.7, 77.1, 77.6, 77.0, 73.6‡ V	Recluse, WY crude	4
	72.9, 73.1, 73.4, 72.4, 67.1# V	Prudhoe Bay, AK crude	5
	76.9§ W	API Crude Oil C	58
	78.0§ W	API Crude Oil D	58
Raw shale oil	41.7 W	Paraho - SOHIO Toledo	35
	70,61,49,44** V	Paraho - SOHIO Gary Western	38
	48.8 W, 60.5 V	In-situ; Rock Springs, WY	35,81
Hydrotreated shale oil	67.4 W	Paraho - SOHIO Toledo	35

Explanatory Notes

*Cycloparaffins in this boiling range are one-, two-, three- and possibly five-ring paraffins.

§Values are for fractions boiling between 350°F and 550°F.

**These values are, respectively, for the following distillation fractions: 380-480°F, 480-520°F, 520-600°F and 600-650°F. These fractions accounted for 5.4, 3.33, 10.09 and 6.67 Vol. percent of crude, respectively.

†Values are for 5 fractions corresponding to 45°F interval cut points of 437, 482, 527, 587 and 637°F and accounting for 3.6, 4.4, 5.3, 4.7 and 6.3 Vol % crude, respectively.

‡Values are for 5 fractions corresponding to 45°F interval cut points of 437, 482, 527, 587 and 637°F and accounting for 4.8, 5.2, 4.8, 4.6 and 6.1 Vol. %, of crude, respectively.

#Values are for 5 fractions corresponding to 45°F interval cut points of 437, 482, 527, 587, 637 °F and accounting for 4.3, 4.8, 5.0, 2.8 and 6.5, Vol. %, respectively.

Table 26. Olefins in Medium Boiling Fractions (approximately 400°F to 650°F)

Material	Value (V = Vol. %; W = Wt. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	19.4 W	Paraho - SOHIO Toledo	35
	3.1,4.6* V	Paraho - SOHIO Gary Western	38
	6.3 W, 11.1 V	In-situ; Rock Springs, WY	35,81
Hydrotreated shale oil	NA	--	--

Explanatory Notes

*Respectively for 380-480°F and 480-520°F distillation fractions. The amounts in the 520-600°F and 600-650°F were outside the limit of available mass spec. instrument. These four fractions accounted, respectively, for 5.4, 3.33, 10.09 and 6.67 Vol. percent of crude.

Table 27. Aromatics[*] in Medium Boiling Fractions (Approximately 400°F to 650°F)

Material	Value (V = Vol. %; W = Wt. %)	Sample Description/Source	Reference
Petroleum crude	22.4,22.2,21.6, 23.8,30.3[†] V	Wilmington, CA crude	4
	19.3,22.8,22.4, 23.0,26.4[‡] V	Recluse, WY crude	4
	27.1,26.9,26.6,[#] 27.6,32.9 V	Prudhoe Bay, AK crude	5
	23.1[§] W	API Crude Oil C	58
	22.0[§] W	API Crude Oil D	58
Raw shale oil[**]	18.8 W	Paraho - SOHIO Toledo	35
	26.9,34.7,50.5 56.4[††] V	Paraho - SOHIO Gary Western	38
	28.5 W,28.4 V[‡‡]	In-situ; Rock Springs, WY	35,81
Hydrotreated shale oil[§§]	29.7 W	Paraho - SOHIO Toledo	35

Explanatory Notes

[*] Aromatics in this boiling range generally consist of mono-, di- and triaromatics (i.e., alkyl benzenes, naphthene benzenes, naphthalenes; and possibly acenaphthalenes, fluorenes, denaphthene benzenes, acenaphthenes and biphenyls). Probable compound types identified by GPC and MS in the 392°F to 617°F boiling range of an ARCO-1 hydrotreated shale oil included: (a) monoaromatics (i.e., alkylbenzenes, alkylindanes and tetralin, and alkly di- through trinaphthenobenezenes); (b) diaromatics (i.e., alkylnaphthalenes, alkyldiphenyl alkanes, alkyl mono-through trinaphthenonaphthalenes and/or alkyl mono- through dinaphthenodiphenylalkanes); and (c) various polyaromatics (see Tables 36 and 37) (Reference 50).

[§] Values are for fractions boiling between 350°F and 550°F.

[**] Triaromatics (aromatics $\geq$3 rings) contents values of 4.7 wt % for a raw shale oil, and none detected for Paraho and in-situ shale oil are reported in Reference 57. Although no temperature range is specified, the data most likely pertain to medium and heavy boiling range fractions (Reference 57).

[††] Values are, respectively, for the following four distillation fractions: 380-480°F, 480-520°F, 520-600°F and 600-650°F. These fractions accounted for 5.4, 3.33, 10.09 and 6.67 Vol. percent of crude, respectively.

[‡‡] Values include sulfur, nitrogen and oxygen compounds.

[§§] The following triaromatics contents are reported for hydrotreated shale materials: 3.7 wt % for a mildly hydrotreated shale oil, 2.1% for a dewaxed syncrude, and none detected for Paraho-SOHIO Toledo hydrotreated shale oil (Reference 57).

[†] Values are for 5 fractions corresponding to 45°F interval cut points of 437, 482, 527, 587 and 637 and acounting for 3.6, 4.4, 5.3, 4.7 and 6.3 Vol. % of crude, respectively.

[‡] Values are for 5 fractions corresponding to 45°F interval cut points of 437, 482, 527, 587 and 637 and accounting for 4.8, 5.2, 4.8, 4.6 and 6.1 Vol. % of crude, respectively.

[#] Values are for 5 fractions corresponding to 45°F interval cut points of 437, 482, 527, 587 and 637 and accounting for 4.3, 4.8, 5.0, 2.8 and 6.5 Vol. % of crude, respectively.

Table 28. Saturates (Paraffins + Napthenes) in Heavy Boiling Fractions (650°F to 850°F)

Material	Value (V = Vol. %; W = Wt. %)	Sample Description/Source	Reference
Petroleum crude	56.3* W	API Crude Oil C	58
	64.2* W	API Crude Oil D	58
Raw shale oil	17.6 W	Paraho - SOHIO Toledo	35
	35.5,37.1,33.2† V	Paraho - SOHIO Gary Western	38
	33.4 W	In-situ; Rock Springs, WY	35
Hydrotreated shale oil	55.5 W	Paraho - SOHIO Toledo	35

Explanatory Notes

*Values are for fractions boiling between 550 and 700°F.

†Values are, respectively, for the following distillation fractions: 650-700°F 700-750°F and 750-800°F. The amount in the 800-843°F were reported outside the detection limits of available mass spec. instrument. These four fractions acounted for 6.21, 6.18, 7.60 and 15.45 Vol. percent of crude, respectively.

Table 29. Olefins in Heavy Boiling Fractions
(650°F to 850°F)

Material	Value (V = Vol. %; W = Wt. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	11.6 W	Paraho - SOHIO Toledo	35
	2* V	Paraho - SOHIO Gary Western	38
	5.4 W	In-situ; Rock Springs, WY	35
Hydrotreated shale oil	NA	--	--

Explanatory Notes

*Value is for each of the following three distillation fractions: 650-700°F, 700-750°F, and 750-800°F. The value for the 800-843°F fraction was reported as outside the detection limits of available mass spec. instrument. These four fractions accounted for 6.21, 6.18, 7.6 and 15.45 Vol. percent of crude, respectively.

Table 30. Aromatics* in Heavy Boiling Fractions
(650°F to 850°F)

Material	Value (V = Vol. %; W = Wt. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	23.0 W	Paraho - SOHIO Toledo	35
	64.5,62.9,66.8† V	Paraho - SOHIO Gary Western	38
	21.8 W	In-situ; Rock Springs, WY	35
Hydrotreated shale oil	38.1 V	Paraho - SOHIO Toledo	35

Explanatory Notes

*Aromatics in this boiling range consist of mono-, di-, tri-, tetra- and pentaaromatics. Probable compound types identifed by GPC and MS in the 617°F to 797°F boiling range of an ARCO-1 hydrotreated shale oil included: (a) monoaromatics (i.e., alkylbenzenes, alkylindans and tetralins, and alkyl di- through hexanaphthenobenzenes); (b) diaromatics (i.e., alkylnaphthalenes, alkyldiphenylalkanes, alkyl mono- through hexanaphthenonaphthalenes and/or alkyl mono- through hexanaphthenodiphenylalkanes); and (c) various polyaromatics (see Table 36, Explanatory Notes) (Reference 50).

†Values are, respectively, for the following three distillation fractions: 650-700°F, 700-750°F and 750-800°F. The value for the 800-843°F fraction was reported as outside of the detection limits of available mass spec. instrument. These four fractions accounted for 6.21, 6.18, 7.6 and 15.45 Vol. percent of crude, respectively.

Table 31. Saturates (Paraffins + Naphthenes) in Residual Boiling Fractions (850°F+)

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum crude	41.2*	API Crude Oil C	58
	42.0*	API Crude Oil D	58
Raw shale oil	7.9	Paraho - SOHIO Toledo	35
	7.0	In-situ; Rock Springs, WY	35
Hydrotreated shale oil	57.3	Paraho - SOHIO Toledo	35

Explanatory Notes

*Values are for fractions boiling between 700-1070°F.

Table 32. Olefins in Residual Boiling Fractions (850°F$^+$)

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	2.6	Paraho - SOHIO Toledo	35
	6.1	In-situ; Rock Springs, WY	35
Hydrotreated shale oil	NA	--	--

Table 33. Aromatics in Residual Boiling Fractions (850°F^{+})

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum crude	56.4*	API Crude Oil C	58
	55.6*	API Crude Oil D	58
Raw shale oil	33.9†	Paraho - SOHIO Toledo	35
	19.6†	In-situ; Rock Springs, WY	35
Hydrotreated shale oil	33.6*	Paraho - SOHIO Toledo	35

Explanatory Notes

*Values are for fractions boiling between 700-1070°F.

*Sulfur-containing compounds are included.

Table 34. Solvent Fractionation - "Type 1"*

Material	Value (Wt. %)		Sample Description/Source	Reference
Petroleum crude	asphaltenes			58
	550-700°F	0.0	API Crude Oil C	
	550-700°F	0.0	API Crude Oil D	
	700-1070°F	0.0	API Crude Oil C	
	700-1070°F	0.0	API Crude Oil D	
	resins			58
	550-700°F	1.2	API Crude Oil C	
	550-700°F	2.9	API Crude Oil D	
	700-1070°F	2.4	API Crude Oil C	
	700-1070°F	2.4	API Crude Oil D	
Raw shale oil	asphaltenes	6.10	Paraho - SOHIO Toledo†	35
	carbenes	0.03		
	carboids	0.01		
	resins	7.40		
	oils	86.46		
	asphaltenes	4.06	In-situ; Rock Springs, WY†	35
	carbenes	0.10		
	carboids	0.41		
	resins	2.96		
	oils	92.47		
	asphaltenes	0.819	Paraho - SOHIO Gary Western	38
	asphaltenes	0.889	Paraho - SOHIO Toledo	33
Hydrotreated shale oil		NA	--	--

Explanatory Notes

*Type 1 Solvent Fractionation is defined as standard SARA separation. Using this method, the asphaltene fraction is that portion of certain crude oil distillation fractions that is insoluble in n-pentane but soluble in benzene. The carbene fraction is that portion of the crude oil distillation fractions that is insoluble in benzene but soluble in carbon disulfide; the carboid fraction is that portion that is insoluble in both benzene and in carbon disulfide. Resins are polar materials in maltenes (that portion of the crude oil distillation fractions that is soluble in n-pentane) that are retained by adsorbents in a standard SARA technique recycle chromatographic column. Oils are resins-free maltenes (References 2 and 59).

†Data were obtained using method of Schwager and Yen (Reference 80), which is a modification of the SARA separation procedure.

Table 35. Solvent Fractionation - "Type 2"*

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	Alkanes: 30 wt%; compounds range from C_8 to C_{32}, with C_{11} and C_{27} having highest concentrations in Kerosene Creek sample. 20-30% are branched alkanes consisting of 2-and 3-methyl alkanes, isoprenoid alkanes, alkyl cyclopentanes and alkylcyclohexanes Alkanes: 10-17 wt %; primarily linear, ranging from C_9 to C_{33}, with C_{10} having the highest concentration in both shale oils. Branched alkanes consisted primarily of pristene isomers, as well as homologous series of 1-alkylcyclohexenes; 2-methyl-3-alkenes and 1-methyl-4-alkylcyclohexenes Aromatics: numerous 1- and 2-phenyl alkanes, polymethyl substituted benzenes, indans, indenes and homologous series of alkylnaphthalenes and 1-phenyl-4-alkenes. Most abundant aromatics were trimethylbenzenes, methylnaphthalenes and ethylnaphthalene	Kerosene Creek, Australia and Ramsay Crossing, Australia shale oils.	60
Hydrotreated shale oil	NA	--	--

Explanatory Notes

*Type 2 Solvent Fractionation is defined as a 10-fraction solvent separation scheme described in Reference 60.

Table 36. PNA Content (Wt. %)

Material	San Joaquin Valley Crude (Ref. 57)	E. Wilmington Crude (Ref. 57)	Southern Louisiana Crude (Ref. 17)
Petroleum crude*,†			
Diaromatics: naphthalenes	2.0	2.0	NA
biphenyls	4.6	4.1	NA
fluorenes	2.8	1.7	NA
Total diaromatics	9.4	7.8	NA
Triaromatics: phenanthrenes	0.3	0	0.033
naph-phenanthrenes	1.6	1.1	--
fluoranthenes	ND	ND	0.00052
Total triaromatics	1.9	1.1	0.033
Tetraaromatics: pyrenes	0.3	0	0.00035
chrysenes	0.7	0.2	0.0018
benzanthracenes	0	0	0.00017
triphenylene	0	0	0.0010
benzofluoranthenes	0	0	<0.00037
Total tetraaromatics	1.0	0.2	<0.0037
Pentaaromatics: benzopyrenes	0	0	0.00033
perylene/benzoperylene	0	0	0.0036
other	0	0	--
Total pentaaromatics	0	0	0.0039
Higher boiling compounds:	1.8	2.9	NA

(Continued)

Table 36 (Continued)

Material	TOSCO-II‡ (Ref. 49)	Paraho (Ref. 31)	In-situ Rock Springs WY§ (Ref. 31)
Raw shale oil			
Diaromatics: naphthalenes	NA	NA	NA
biphenyls	NA	NA	NA
fluorenes	NA	<0.0029	0.036
Total diaromatics	NA	<0.0029	0.036
Triaromatics: phenanthrenes	NA	0.0077	0.26
naph-phenanthrenes	NA	NA	NA
fluoranthenes	0.00069, 0.00037, ND	0.00047	0.034
other	NA	0.0011	0.047
Total triaromatics	0.00069, 0.00037, ND	0.0093	0.341
Tetraaromatics: pyrenes	0.0019, 0.0031, 0.0027	0.00026	0.050
chrysenes	0.00056, 0.00069, 0.00054	<0..00046	0.015
benzanthracenes	0.00027, 0.00045, 0.00021	0.0018	0.021
triphenylene	0.00013, 0.00020, 0.00019	<0.00065	0.0031
benzofluoranthenes	NA	<0.0032	0.0094
Total tetraaromatics	0.0029, 0.0044, 0.0036	<0.0064	0.099
Pentaaromatics: benzopyrenes	0.00045, 0.00095, 0.00065	<0.0016	0.017
perylene/benzoperylene	0.00015, 0.000072, ND	<0.00061	0.001
other	0.00005, ND , ND	<0.0005	0.0007
Total pentaaromatics	0.00065, 0.00095, 0.00065	<0.0027	0.019
High boiling compounds:	NA	NA	NA

(Continued)

Table 36 (Continued)

Material	TOSCO-II‡ (Ref. 49)	Paraho (Ref. 31)
Hydrotreated shale oil#		
Diaromatics: naphthalenes	NA	NA
biphenyls	NA	NA
fluorenes	NA	0.0028
Total diaromatics	NA	0.0028
Triaromatics: phenanthrenes	NA	0.013
naph-phenanthrenes	NA	NA
fluoranthenes	0.00098, 0.00016, ND	0.0023
other	NA	<0.0010
Total triaromatics	0.00098, 0.00016, ND	<0.016
Tetraaromatics: pyrenes	0.0175, 0.1090, 0.0715	0.015
chrysenes	0.000092,0.00056, 0.00035	0.0016
benzanthracenes	NA , 0.00018, 0.00014	0.0040
triphenylene	NA , 0.00017, 0.00025	0.0002
benzofluoranthenes	NA	0.0135
Total tetraaromatics	0.0021, 0.013 , 0.008	0.035
Pentaaromatics: benzopyrenes	0.00038, 0.00092, 0.00012	0.0107
perylene/benzoperylene	0.0014 , 0.00085, 0.00027	0.0080
other	0.00008, ND , ND	0.0010
Total pentaaromatics	0.0018 , 0.0018 , 0.00039	0.020
Higher boiling compounds:	NA	NA

(Continued)

Table 36. PNA Content (Wt. %) (Continued)

Material	Mildly Hydrotreated (Ref. 57)	Dewaxed Syncrude (Ref. 57)
Diaromatics: naphthalenes	1.4	0.4
biphenyls	2.4	1.0
fluorenes	1.2	0.6
Total diaromatics	5.0	2.0
Triaromatics: phenanthrenes	0.9	0.6
naph-phenanthrenes	0.5	0.4
fluoranthenes	NA	NA
Total triaromatics	1.4	1.0
Tetraaromatics: pyrenes	0.6	0.4
chrysenes	0.4	0.3
benzanthracenes	NA	NA
triphenylene	NA	NA
benzofluoranthenes	NA	NA
Total tetraaromatics	1.0	0.7
Total pentaaromatics	0.4	0.2
Higher boiling compounds	0.9	0.2

(Continued)

Table 36 (Concluded)

Explanatory Notes

*Polynuclear aromatics contents of 4.9 wt % and 2.1 wt % have been reported for API Crude Oils C and D, respectively, in the 700 - 1000°F distillation cut. PNA contents of 2.6 wt. % and 1.8 wt. % were reported for the 550-700°F distillation cuts, respectively. Extremely low levels (<0.00003 wt %) of tri- and tetraaromatic PNA's were found in the 130-350°F and 350-550°F distillation cuts for these oils (Reference 58).

†Under API Project PS-8-GST-(989-300), the following polynuclear aromatics contents were found in the high boiling (700-1070°F) distillation cut sample and the oil and aromatics fraction obtained by the SARA separation procedure of two petroleum crudes: 0.0128 and 0.0063 wt. % (original cut); 0.0175 and 0.0071 wt. % (oil fraction); and 0.0354 and 0.0121 wt. % (aromatics fraction). PNA contents of the comparable intermediate boiling (550-700°F) distillation cuts and SARA fractions were: 0.0054 and 0.0002 wt. % (original cut); 0.0095 and 0.0028 wt. % (oil fraction), and 0.02 and 0.0067 wt. % (aromatics fraction). The medium boiling (350-550°F) cut, oil fraction of one of the crudes contained the following PNA concentrations: 0.002 wt. % fluorene, <0.0001 wt. % pyrene, <0.0001 wt. % fluoranthenes, 0.0002 wt. % phenanthrenes and 0.0032 wt. % methyl phenanthrenes. The low boiling (120 to 350°F) cut of a third crude contained 0.0006 wt. % pyrene, and <0.0001 wt. % of benza(a)anthracene, benzo(a)pyrene and benzo(g,h,i) perylene (Reference 79).

‡TOSCO-II values are for 3 paper chromatographic fractions; i.e., PAH, alkyl PAH-I and alkyl PAH-II, respectively.

§In-situ Rock Springs WY values are averages of two samples.

#Probable PNA compound types identified by GPC/MS in the 617° to 797°F boiling range of an ARCO-1 hydrotreated shale oil include: (1) alkylacenaphthalenes and fluorenes, (2) naphtheno derivations of (1) and/or alkylphenanthrenes and alkylanthracenes; (3) naphtheno derivatives of (2); (4) naphtheno derivatives of (3) and/or alkylpyrenes/fluoranthenes/benzanthrenes; and (5) naphtheno derivatives of (4) and/or alkylchrysenes/benzophenanthrenes (Reference 50).

Table 37. Distribution of PNA Compound Types by Mass Spectrometric Z Number (Wt T)*

A. Monoaromatic Concentrates (698-995°F)

Material	Mass Z Series	Prudhoe Bay, AK	Gach Saran	Swan Hills, CA	Wilmington, CA	Recluse, WY	Probable Compound Type	Reference
Petroleum crude	-4	0.01	ND	ND	ND	ND	Alkyltrinaphthenes.	4
	-6	12.60	13.36	10.56	4.61	9.11	Alkylbenzenes.	
	-8	16.77	15.55	14.85	12.96	14.99	Alkylnaphthenobenzenes.	
	-10	16.97	16.11	17.14	16.67	15.59	Alkyldinaphthenobenzenes.	
	-12	16.91	13.68	15.63	16.92	13.48	Alkyltrinaphthenobenzenes.	
	-14	14.31	12.30	14.34	13.88	12.31	Alkyltetranaphthenobenzenes.	
	-16	9.88	9.00	10.95	9.71	9.22	Alkylpentanaphthenobenzenes.	
	-18	6.71	6.35	7.23	6.02	6.81	Alkylhexanaphthenobenzenes.	
	-20	1.34	.68	2.36	2.47	3.16	Alkylheptanaphthenobenzenes.	
	-22	0.27	0.2	.70	.70	.27	Alkyloctanaphthenobenzenes.	
	-24	ND	ND	.02	ND	ND	Alkylnonanaphthenobenzenes.	
	-12	ND	ND	.94	1.42	3.67	Alkylnaphthalenes.	
	-14	ND	.02	.90	1.44	3.16	Alkylnaphthenonaphthalenes and/or aklyldiphenylalkanes.	
	-16	ND	.04	.79	.76	2.34	Alkyldinaphthenonaphthalenes and/or alkylnaphthenodiphenylalkanes.	
	-18	ND	.02	.38	.47	.80	Alkyltrinaphthenonaphthalenes and/or alkyldinaphthenodiphenylalkanes.	
Raw shale oil				NA			--	--
Hydrotreated shale oil				NA			--	--

(Continued)

Table 37 (Continued)

B. Diaromatic Concentrates (698-995°F)

Material	Mass Z Series	Prudhoe Bay, AK	Gach Saran	Swan Hills, CA	Wilmington, CA	Recluse WY	Probable Compound Type	Reference
Petroleum crude	-12	3.83	2.54	2.90	4.72	4.68	Alkylnaphthalenes.	4
	-14	13.84	14.86	11.84	13.75	13.52	Alkylnaphthenonaphthalenes and/or alkylbiphenyls or diphenylalkanes.	
	-16	18.53	15.79	18.87	18.62	15.87	Alkyldinaphthenonaphthalenes and/or alkylnaphthenobiphenyls or naphthenodiphenylalkanes.	
	-18	15.61	13.57	19.25	12.69	16.52	Alkyltrinaphthenonaphthalenes and/or alkyldinaphthenobiphenyls or dinaphthenodiphenylalkanes.	
	-20	8.66	5.84	14.48	7.19	16.10	Alkyltetranaphthenonaphthalenes and/or alkyltrinaphthenobiphenyls or trinaphthenodiphenylakanes.	
	-22	5.78	3.03	11.04	3.68	11.80	Alkylpentanaphthenonaphthalenes and/or alkyltetranaphthenobiphenyls or tetranaphthenodiphenylalkanes.	
	-24	4.45	.46	7.60	2.57	7.27	Alkylhexanaphthenonaphthalenes and/or alkylpentanaphthenobiphenyls or pentanaphthenodiphenylalkanes.	
	-26	.98	ND	4.22	ND	3.80	Alkylheptanaphthenonaphthalenes and/or alkylhexanaphthenobiphenyls or hexanaphthenodiphenylalkanes.	
	-28	ND	ND	1.43	ND	1.01	Alkyloctanaphthenonaphthalenes and/or alkylheptanaphthenobiphenyls or heptanaphthenodiphenylalkanes.	
	-8	ND	ND	.26	ND	ND	Alkylnaphthenobenzenes.	
	-10	ND	ND	.40	ND	ND	Alkyldinaphthenobenzenes.	
	-16	ND	ND	ND	ND	1.95	Alkylacenaphthalenes.	
	-18	ND	ND	ND	ND	1.87	Alkylnaphthenoacenaphthalenes.	
	-20	ND	ND	ND	ND	.41	Alkyldinaphthenoacenaphthalenes.	
Raw shale oil				NA			--	--
Hydrotreated shale oil				NA			--	--

(Continued)

Table 37 (Concluded)

C. Polyaromatic-Polar Concentrates (668-995°F)

Material	Mass Z Series	Prudhoe Bay, AK	Gach Saran	Swan Hills, CA	Wilmington, CA	Recluse, WY	Probable Compound Type	Reference
Petroleum crude	-16	3.11	.84	2.33	3.90	1.98	Alkylbenzoindenes.	4
	-18	7.33	4.40	6.78	8.38	6.19	Alkylnaphthenobenzoindenes and/or alkylphenanthrenes/anthracenes	
	-20	11.83	7.08	11.52	8.70	12.85	Alkyldinaphthenobenzoindenes and/or alkylnaphthenophenanthrenes/anthracenes and/or alkylphenylnaphthalenes and/or alkyldiacenaphthalenes	
	-22	11.13	4.75	15.34	8.47	16.13	Alkyltrinaphthenobenzoindenes and/or alkyldinaphthenophenanthrenes/anthracenes and/or alkylnaphthenophenylnaphthalenes and/or alkyldibenzoindenes	
	-24	8.67	3.93	13.69	6.56	15.82	Alkyltetranaphthenobenzoindenes and/or alkyltrinaphthenophenanthrenes/anthracenes and/or alkyldinaphthenophenylnaphthalenes and/or alkylnaphthenodibenzoindenes	
	-26	5.60	ND	9.93	2.62	12.48	Alkylpentanaphthenobenzoindenes and/or alkyltetranaphthenophenanthrenes/ anthracenes and/or alkyltrinaphthenophenylnaphthalenes and/or alkyldinaphthenodibenzoindenes	
	-28	3.81	ND	6.61	1.35	9.69	Alkylheptanaphthenobenzoindenes and/or alkylpentanaphthenophenanthrenes/anthracenes and/or alkyltetranaphthenophenylnaphthalenes and/or alkyldinaphthenodibenzoindenes	
	-30	1.30	ND	3.91	.21	6.46	Alkylheptanaphthenobenzoindenes and/or alkylhexanaphthenophenanthrenes/ anthracenes and/or alkylpentanaphthenophenylnaphthalenes and/or alkyltetranaphthenodibenzoindenes	
	-32	.76	ND	3.42	.42	5.16	Alkyloctanaphthenobenzoindenes and/or alkylhexanaphthenophenylnaphthalenes and/or alkylpentanaphthenodibenzoindenes	
	-34	.05	ND	.46	ND	1.25	Alkylheptanaphthenophenylnaphthalenes and/or alkylhexanaphthenodibenzoindenes	
	-36	ND	ND	ND	ND	.24	Alkyloctanaphthenophenylnaphthalenes and/or alkylheptanaphthenodibenzoindenes	
	-16	ND	ND	ND	ND	.32	Alkyldinaphthenonaphthalenes	
Raw shale oil			NA				--	--
Hydrotreated shale oil			NA				--	--

Table 38. Individual Nitrogen-Containing Compounds

Material		Value (wt %)	Sample Description/Source	Reference
Petroleum crude		NA	--	--
Raw shale oil	Compound*	Wt% in X-215°C Fraction	Wt% in Full-Range Shale Oil	57
	Pyridines			
	C1	0.04	0.003	
	C2	0.36	0.032	
	C3	1.27	0.111	
	C4	0.84	0.074	
	C5	0.73	0.064	
	C6	0.15	0.013	
	Pyrroles			
	C2	0.05	0.004	
	C3	0.05	0.004	
	Methyl Phenyl Acetamide	0.04	0.003	
	Unknown	0.51	0.045	
	Total	4.04	0.353	

(Continued)

Table 38 (Continued)

Material	Value (wt %)		Sample Description/Source		Reference
Hydrotreated shale oil	NA	NA	NA		--
	Dearsenited Shale Oil		Dewaxed Syncrude		57
Compound	Wt% in X-215°C Fraction	Wt% in Full-Range Shale Oil	Wt% in X-215°C Fraction	Wt% in Full-Range Shale Oil	
Pyridines					
C_1	<0.01	<0.001	Insufficient Extractable Material to Test		
C_2	0.11	0.013			
C_3	0.60	0.068			
C_4	0.94	0.106			
C_5	1.06	0.120			
C_6	0.30	0.034			
Pyrroles					
C_2	0.09	0.010			
C_3	0.09	0.010			
Methyl Phenyl Acetamide	0.01	0.001			
Unknown	0.69	0.078			
Total	3.89	0.440			

(Continued)

Table 38 (Concluded)

Explanatory Notes

*Based on data obtained in other studies for the light boiling (i.e., naphtha) distillation fractions of raw shale oils from Colorado, Scotland, Australia, Manchuria and Russia; the following are likely specific constituents comprising C_1 - C_6 pyridines, C_2 and C_3 pyrroles, etc. (Reference 29).

Pyridines

C_1: 2-,3- and 4-methyl pyridine

C_2: 2,3-; 2,4-; 2,5-; 2,6-; 3,4-; and 3,5-dimethyl pyridine and 2-,3-, and 4-ethylpyridine

C_3: 2,3,5-; 2,3,6-; 2,4,5-; and 2,4,6-trimethyl pyridine and 2-methyl-4-ethyl, 4-methyl-2-ethyl, 2-methyl-5-ethyl, 2-methyl-6-ethyl, and 4-methyl-3-ethyl pyridine.

C_4: 2,3,4,5-; 2,3,4,6-; and 2,3,5,6-tetramethylpyridine and 2,6-dimethyl-4-ethyl, 2,4-dimethyl-6 ethyl, and 2,4-diethyl pyridine, 2-butylpyridine, quinoline and isoquinoline.

Pyrroles

C_1: 2-methylpyrrole

C_3: 2,3,5-trimethylpyrrole

Others

Pyrrole, dihydropyridine, 2,3,4,5-tetramethylpyrrole; 2,3,5-trimethyl-3-ethylpyrrole; benzonitrile; 2- and 3-methylbenzonitrile, hexanenitrile, heptanenitrile and octanenitrile.

Table 39. Distribution of Nitrogen Content by Mass Spectrometric Z Number

		Value†			
Material	Z No	Carbon Number Range	Carbon Number Having Greatest Concentration and Concentration (ppmw)	Sample Description Source	Reference
Petroleum crude*	-3	C_{12}	C_{12} (3)	San Joaquin Valley crude	57
	-5	C_8-C_{13}	C_9 (20)		
	-7	C_8-C_{20} (exc. $C_{9,16}$)	C_{12} (30)		
	-9	C_8-C_{24} (exc.C_{22})	C_{16} (40)		
	-11	C_{11}-C_{24}	C_{17}, C_{19} (60)		
	-13	C_{12}-C_{26}	C_{18}, C_{19} (60)		
	-15	C_{13}-C_{27}	C_{17} (150)		
	-17	C_{13}-C_{27}	C_{18} (200)		
	-19	C_{13}-C_{27} (exc. C_{15})	C_{22} (120)		
	-21	C_{17}-C_{27}	C_{19} (210)		
	-23	C_{18}-C_{27}	C_{25} (110)		
	-25	C_{17}-C_{27} (exc. $C_{20,\ 21}$)	C_{26} (90)		
	-27	C_{19}, C_{24}-C_{27}	C_{25} (60)		
	-3	ND	ND	E. Wilmington crude	57
	-5	C_8-C_{19}	$C_{8,\ 9,\ 10}$ (20)		
	-7	C_{10}-C_{21}	C_{12} (40)		
	-9	C_{10}-C_{23}	C_{17} (40)		
	-11	C_{11}-C_{25}	C_{17} (60)		
	-13	C_{12}-C_{27}	C_{20} (50)		
	-15	C_{12}-C_{27}	C_{16} (300)		
	-17	C_{15}-C_{27}	C_{20} (170)		
	-19	C_{15}-C_{27}	C_{23} (120)		
	-21	C_{15}-C_{27}	C_{19} (180)		
	-23	C_{18}-C_{25} (exc. $C_{20,21}$)	$C_{22,\ 23}$ (80)		
	-25	C_{18}, C_{22}	C_{22} (40)		
	-27	ND	ND		
Raw shale oil	NA	NA	NA	--	--
Hydrotreated shale oil	NA	NA	NA	--	--

(Continued)

Table 39 (Concluded)

Material	Z No	Value† Carbon Number Range	Carbon Number Having Greatest Concentration and Concentration (ppmw)	Sample Description/Source	Reference
	-3	C_8-C_{20} (exc. C_{15})	$C_{8,9}$(30)	Mildly hydrotreated shale oil	57
	-5	C_8-C_{22}	C_8(1130)		
	-7	C_8-C_{22}	C_{12}(380)		
	-9	C_9-C_{22}	C_{12}(570)		
	-11	C_{10}-C_{22}	$C_{13,14}$(300)		
	-13	C_{11}-C_{22}	C_{15}(210)		
	-15	C_{12}-C_{22}	C_{15}(220)		
	-17	C_{14}-C_{22}	C_{17}(90)		
	-19	C_{15}-C_{22}	$C_{17,18,19}$(40)		
	-21	C_{16}-C_{22} (exc. C_{18})	$C_{17,20,21}$(30)		
	-23	C_{19}-C_{22}	$C_{21,22}$(20)		
	-25	C_{19}-C_{22}	$C_{20,21,22}$(10)		
	-27	ND	ND		
	-3	C_8-C_{12} (exc. $C_{9,10}$)	C_8(4)	Dewaxed full-range syncrude	
	-5	C_9,C_{11},C_{12},C_{16}	C_{12}(3)		
	-7	C_{11},C_{12},C_{14}	C_{11},C_{12},C_{14}(2)		
	-9	ND	ND		
	-11	ND	ND		
	-13	ND	ND		
	-15	C_{12},C_{14},C_{15}	C_{15}(4)		
	-17	C_{15},C_{16}	C_{16}(10)		
	-19	C_{14},C_{15}	C_{14},C_{15}(2)		
	-21	ND	ND		
	-23	ND	ND		
	-25	ND	ND		
	-27	ND	ND		

Explanatory Notes

*Mass spectrographic operating conditions used not specified.

†Data indicate higher concentrations of nitrogen compounds in the lower molecular weight (i.e., C_8-C_{16}) region for the shale materials, and higher concentrations in the higher molecular weight (C_{18}-C_{27}) region for crudes.

Table 40. Relative Distribution of N-PNA Compound Types by Mass Spectrometric Z Number

Material	Z No.	Nominal Structures	Value*		Sample Description/Source	Reference
Petroleum crude	NA	NA	NA		--	--
Raw shale oil	-3	Pyrroles	0.9	0.3	Paraho-SOHIO Toledo, (Column 1): In-situ, Rock Springs, WY (Column 2)	31
	-5	Pyridines	13	4		
	-7	Azaindanes	5	2		
	-9	Indoles	16	24		
	-11	Quinolines	6	5		
	-13	Phenyl pyridines	4	3		
	-15	Carbazoles	19	26		
	-17	Acridines	9	15		
	-19	Benzo(d,e,f)carbazoles	6	4		
	-21	Azapyrenes, Benzcarbazoles	8	10		
	-23	Benzacridines	3	3		
	-27	Dibenzacarbazoles	2	1.3		
	-29	Dibenzacridines	3	0.2		
Hydrotreated shale oil†	-3	Pyrroles	0		Paraho-SOHIO, Toledo	31
	-5	Pyridines	21			
	-7	Azaindanes	6			
	-9	Indoles	8			
	-11	Quinolines	8			
	-13	Phenyl pyridines	7			
	-15	Carbazoles	20			
	-17	Acridines	7			
	-19	Benzo(d,e,f)carbazoles	4			
	-21	Azapyrenes, Benzcarbazoles	11			
	-23	Benzacridines	3			
	-27	Dibenzcarbazoles	0.9			
	-29	Dibenzacridines	0.4			

Explanatory Notes

*Only nitrogen-containing masses were examined in the samples, and the data are normalized to 100% (wt/wt) in order to determine relative compound distributions.

†Probable nitrogen-containing compound types identified by GPC and MS in the 392-617°F boiling range of an ARCO-1 hydrotreated shale oil included: (a) alkylcarbazoles; (b) alkylnaphthenocarbazoles; and (c) alkylnaphthenocarbazoles. Alkylcarbazoles and alkylnaphthenocarbazoles were also identified in the 617-797°F boiling range (Reference 50).

Table 41. Compound Class Analysis - Solvent Fractionation ("Type 1")*

Material	Value (% Recovery)	Sample Description/Source	Reference
Petroleum crude	NA	--	--
Raw shale oil	saturates - 31.7 aromatics - 11.2 N-heterocyclics - 15.1 (non-basic) N-heterocyclics - 17.9 (basic) Polars - 15.8 Loss (volatiles) - 8.3	Paraho-SOHIO Toledo	31
	saturates - 32.2 aromatics - 14.5 N-heterocyclics - 8.1 (non-basic) N-heterocyclics - 16.3 (basic) Polars - 11.0 Loss (volatiles) - 17.9	In-situ; Rock Springs, WY	31
Hydrotreated shale oil	saturates - 66.5 aromatics - 9.8 N-heterocyclics - 2.5 (non-basic) N-heterocyclics - 2.9 (basic) Polars - 0.9 Loss (volatiles) - 17.4	Paraho-SOHIO Toledo	31

Explanatory Notes

*This type of solvent fractionation involves a combination of chromatography on silicic acid and liquid-liquid extraction with N-methylpyrrolidine, as described in Reference 30.

Table 42. Compound Class Analysis - Solvent Fractionation ("Type 2")*

A. Compound Type Fractions and Elemental Nitrogen Content of Fractions

Material	Hydrocarbon		Pyridine I		Pyrrole		Pyrrole/Arylamine		Pyridine II	
	wt % of sample	N, wt % of fraction	wt % of sample	N, wt % of fraction	wt % of sample	N, wt % of fraction	wt.% of sample	N, wt.% of fraction	wt % of sample	N. wt % of fraction
Petroleum crude	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Raw shale oil	31.7	0.003	16.9	1.22	3.56	1.10	5.47	3.92	19.2	4.11
	54.3	0.005	12.2	1.38	1.88	3.57	4.75	3.48	8.72	4.65
Hydrotreated shale oil	81.6	<0.001	2.84	4.51	0.48	0.34	2.54	4.65	2.88	5.91
	87.9	<0.001	0.61	2.80	NA	NA	NA	NA	NA	NA
	93.2	<0.001	0.24	3.94						
	69.3	0.004	9.79	1.99	0.50	0.62	2.58	3.68	3.46	4.12
	79.1	0.002	7.34	1.96	0.73	1.62	2.16	4.75	2.79	4.66
	85.7	0.002	3.91	2.11	0.18	0.52	0.94	4.90	0.99	5.58

(Continued)

Table 42 (Continued)

B. Potentiometric Titration Results for Compound Type Fractions

		Nitrogen, Wt. % of Fraction								
Material	Nitrogen Compound Types	Strong Base pKa 9 to 11	Weak Base pKa 7 to 9	Weak Base II pKa 4 to 7	Weak Base II pKa 2 to 7	Very Weak Base pKa-1 to 2	Nonbasic Nitrogen Compounds	Total	Sample Description/Source	Reference
Petroleum crude	NA	NA	NA	NA	NA	NA	NA	NA	--	--
Raw shale oil	Hydrocarbon	ND	1.07	ND	ND	0.65	0.47	2.19	Paraho-SOHIO†	32
	Pyridine I	ND	0.90	ND	ND	0.19	0.13	1.22		
	Pyrrole	ND	ND	0.17	ND	0.23	0.70	1.10		
	Pyrrole/ Arylamine	ND	ND	0.37	ND	0.96	2.59	3.92		
	Pyridine II	ND	2.77	ND	ND	0.36	0.98	4.11		
	Amide	ND	1.11	ND	ND	1.70	1.72	4.53		
Hydro-treated shale oil	Hydrocarbon	ND	0.29	0.02	ND	0.07	0.05	0.43	Paraho-SOHIO†	32
	Pyridine II	ND	3.46	ND	ND	ND	1.05	4.51		
	Pyrrole	ND	ND	ND	ND	0.13	0.21	0.34		
	Pyrrole/ Arylamine	ND	ND	0.17	0.09	1.13	3.26	4.65		
	Pyridine II	ND	5.46	ND	ND	0.45	ND	5.91		
	Amide	0.20	2.64	1.01	ND	1.48	0.67	6.00		

(Continued)

Table 42 (Continued)

C. Nitrogen-Compound Type Fraction Distribution

Nitrogen, wt. % of Sample

		Weak Base I		Weak Base II		Weak Base II		Very Weak Base	
Material	Strong Base alkylamines	Hindered alkylpyridines/alkylquinolines	Alkylquinolines/alkylpyridines/alkylacridines	Alkylphenanthridines	Hydroquinolines/hydroindoles	Alkylanilines	Hindered alkylanilines	Unknown	Hydroxypyridines
Petroleum crude	NA	NA	NA	NA	NA	NA	NA	NA	NA
Raw shale oil	ND	0.153	0.762	0.020	0.006	ND	ND	0.032	0.423
	0.012	0.127	0.626	0.044	0.010	ND	ND	0.031	0.223
Hydrotreated shale oil	0.001	0.098	0.169	0.004	0.004	0.002	ND	ND	0.020
	trace	0.015	0.026	0.007,	0.001,	0.004	ND	trace	0.003
	trace	0.007	0.010	0.003	<0.001	0.001	ND	trace	0.002
	0.011	0.175	0.245	ND	0.021	0.043	0.017	ND	0.053
	trace	0.132	0.172	ND	0.020	0.022	0.010	0.002	0.018
	trace	0.076	0.063	ND	0.009	0.011	ND	0.003	0.009

(Continued)

Table 42 (Concluded)

C. Nitrogen-Compound Type Fraction Distribution

Material	Very Weak Base (cont'd)	Nonbasic				Sample Description/Source	Reference
	Alkylpyrroles/ alkylindoles	N-alkylcarbazoles/ porphyrins	Alkylcarbazoles	Carboxamide	Total		
Petroleum crude	NA	NA	NA	NA	NA	--	--
Raw shale oil	0.061	0.024	0.166	0.546	2.193	Paraho-SOHIO	32
	0.053	0.011	0.126	0.155	1.418	Modified in-situ, Occidental	32
Hydrotreated shale oil	0.029	0.030	0.084	0.003	0.444	Paraho-SOHIO	32
	0.008	0.001	0.023	0.002	0.090	Paraho-Chevron	32
	0.004	0.002	0.018	0.005	0.052		
	0.044	0.002	0.043	0.029	0.683	Modified in-situ, Occidental; LETC	32
	0.044	ND	0.040	0.008	0.468		
	0.013	0.003	0.030	0.016	0.233		

Explanatory Notes

*This solvent fractionation method involves separation of the sample into six compound-type fractions using basic/neutral alumina and silica adsorption chromatography; method is described in References 32 and 53.

†The results for the Paraho shale oil and Paraho-SOHIO hydrotreated shale oil are typical of those obtained from the Occidental modified in-situ raw shale oil, the Paraho-Chevron hydrotreated shale oil and the Occidental-LETC hydrotreated shale oil.

Table 43. N-PNA Compound Class and Type Analysis - Solvent Fractionation ("Type 2") and High Resolution Mass Spectrometric Analysis (Ref. 53)

A. Pyridine I, Pyridine II and Amide/Pyridine III Fractions

				Compound-type fractions					
				Pyridine I		Pyridine II		Amide/ pyridine III	
Material	Sample Description/ Source	Series empirical formula	Suggested compound types	Percent ioni- zation of parent series reported	Carbon no. range	Percent ioni- zation of parent series reported	Carbon no. range	Percent ioni- zation of parent series reported	Carbon no. range
Petroleum crude	NA	NA	NA	NA	NA	NA	NA	NA	NA
Raw shale oil	NA	NA	NA	NA	NA	NA	NA	NA	NA
Hydrotreated shale oil	Paraho-SOHIO Toledo	$C_nH_{2n+1}N$	Alkylpiperidines/ alkylpyrrolidines	ND	ND	ND	ND	32	7 to 27
		$C_nH_{2n-1}N$	Alkyltetrahydro- pyridines/alkyl- naphthenopiperidines	ND	ND	ND	ND	19	7 to 25
		$C_nH_{2n-3}N$	Alkyldihydropyri- dines	ND	ND	ND	ND	8	7 to 21
		$C_nH_{2n-5}N$	Alkylpyri- dines	48	7 to 35	27	7 to 31	8	7 to 19
		$C_nH_{2n-7}N$	Alkylnaphtheno- pyridines	21	7 to 35	22	7 to 31	8	7 to 19
		$C_nH_{2n-9}N$	Alkyldinaphtheno- pyridines	6	8 to 32	16	7 to 31	7	8 to 20
		$C_nH_{2n-11}N$	Alkylquino- lines	7	10 to 29	11	9 to 28	ND	ND
		$C_nH_{2n-13}N$	Alkylnaphtheno- quinolines	4	10 to 30	8	10 to 28	ND	ND
		$C_nH_{2n-15}N$	Alkyldinaphtheno- quinolines	2	12 to 35	7	11 to 28	ND	ND

(Continued)

Table 43 (Continued)

A. Pyridine I, Pyridine II and Amide/Pyridine III Fractions (Continued)

Material	Sample Description/ Source	Series empirical formula	Suggested compound types	Compound-type fractions					
				Pyridine I		Pyridine II		Amide/ pyridine III	
				Percent ionization of parent series reported	Carbon no. range	Percent ionization of parent series reported	Carbon no. range	Percent ionization of parent series reported	Carbon no. range
Hydrotreated shale oil	Paraho-SOHIO Toledo	$C_nH_{2n-17}N$	Alkylacridines/ alkylphenanthridines	ND	ND	3	14 to 27	ND	ND
		$C_nH_{2n-19}N$	Alkylnaphthenoacridines	ND	ND	2	14 to 26	ND	ND
		$C_nH_{2n-14}N_2$	Alkyldiazaaromatics	ND	ND	ND	ND	1	16 to 22
		$C_nH_{2n-1}NO$	Alkylpiperidones/ alkylpyrrolidones	ND	ND	ND	ND	1	7 to 13
		$C_nH_{2n-3}NO$	Alkylhydroxypyrroles	ND	ND	ND	ND	2	6 to 16
		$C_nH_{2n-5}NO$	Alkylhydroxypyridines	ND	ND	ND	ND	1	7 to 15
		$C_nH_{2n-7}NO$	Alkylbenzamides/ alkylacetylpyridines	ND	ND	1	8 to 20	2	7 to 24
		$C_nH_{2n-9}NO$	Alkylhydroxyindoles	ND	ND	2	9 to 17	2	11 to 20
		$C_nH_{2n-11}NO$	Alkylhydroxyquinolines/alkylacetylindoles	ND	ND	1	11 to 16	1	16 to 20
		$C_nH_{2n-8}N_2O_2$	Unknown	2	7 to 33	ND	ND	ND	ND
		$C_nH_{2n-10}N_2O_2$	Unknown	3	10 to 23	ND	ND	ND	ND

(Continued)

Table 43 (Concluded)

B. Pyrrole and Pyrrole/Arylamine Fractions

				Compound-type fractions			
				Pyrrole		Pyrrole/arylamine	
Material	Sample Description/ Source	Series empirical formula	Suggessted compound types†	Percent ionization of parent series reported	Carbon no. range	Percent ionization of parent series reported	Carbon no. range
Petroleum crude	NA	NA	NA	NA	NA	NA	NA
Raw shale oil	NA	NA	NA	NA	NA	NA	NA
Hydrotreated shale oil	Paraho-SOHIO Toledo	$C_nH_{2n-7}N$	Alkylnaphthenoanilines/ alkylhydroindoles	ND	ND	2	7 to 23
		$C_nH_{2n-9}N$	Alkylindoles	17	8 to 23	7	9 to 21
		$C_nH_{2n-11}N$	Alkylnaphthenoindoles/ alkyltetrahydrocarbazoles	4	9 to 19	3	9 to 18
		$C_nH_{2n-15}N$	Alkylcarbazoles	30	12 to 33	30	11 to 32
		$C_nH_{2n-17}N$	Alkylnaphthenocarbazoles	6	13 to 30	16	13 to 30
		$C_nH_{2n-19}N$	Alkyldinaphthenocarbazoles	ND	ND	7	11 to 28
		$C_nH_{2n-21}N$	Alkylbenzocarbazoles/ alkyltriphenylamines	ND	ND	11	15 to 27
		$C_nH_{2n-23}N$	Alkylnaphthenobenzocarbazoles	ND	ND	6	15 to 28
		$C_nH_{2n-25}N$	Alkyldinaphthenobenzocarbazoles	ND	ND	4	15 to 26
		$C_nH_{2n-x}N_2$	Alkyldiazaaromatics	ND	ND	trace	16 to 22
		$C_nH_{2n-x}NO_2$	Unknown	ND	ND	trace	9 to 18
		$C_nH_{2n-9}NO$	Alkylhydroxyindoles	2	10 to 15	1	8 to 13
		$C_nH_{2n-11}NO$	Alkylhydroxyquinolines/ alkylacetylindoles	1	10 to 14	ND	ND

Explanatory Notes

*This solvent fractionation method involves separation of the sample into 6 compound-type fractions using basic/neutral alumina and silica gel adsorption chromatography and is described in Reference 32 and 53 (See Table 42).

†Not included in this table are the suggested compound types in the pyrrole/arylamine fraction such as the naphthenobenzologs of aniline represented by the series $C_nH_{2n-x}N$ (x = odd, 7 to 25).

Table 44. Compound Class Analysis: Solvent Fractionation - "Type 3"

Material	Fraction Description	Sample Description/Source	Reference
Petroleum crude	NA	---	--
Raw shale oil	Aliphatic nitriles: compounds range from C_9 to C_{34}, with C_{18} and C_{28} having highest concentrations, for Kerosene Creek oil; same for Ramsay Crossing oil, except first highest concentration at C_{19} rather than C_{18}; this fraction accounts for $\geq$20% of the total wt % of nitrogen in the shale oil. Amides: 15 wt % of Kerosene Creek and 7 wt % of Ramsays Crossing shale oils, respectively. Kerosene Creek sample contained homologous series of straight-chain alkamides and 2-methyl-alkanamides ranging from C_9 to C_{28}. Ramsays Crossing sample too complex to be resolved. Basic compounds: 16 wt % of Kerosene Creek and 20 wt % of Ramsay Crossing shale oils; consists of methyl substituted pyridines and quinolines in the low M.W. portion of the fraction, and numerous higher nitrogen heterocycles in the higher M.W. portion of the fraction.	Kerosene Creek, Australia and Ramsay Crossing Australia shale oils	60
Hydrotreated shale oil	NA	--	--

Explanatory Notes

*This solvent fractionation method is defined as a 10-fraction solvent separation scheme described in Reference 60.

Table 45. Sulfur- and Oxygen-Containing Compound Types Identified by High Resolution Mass Spectrometry*

Material	Compound Type	Total Ion Fraction	Estimated Concentration	Sample Description/Source	Reference
Petroleum crude	Hydrocarbons	.54	Approx. 10 percent aromatics	API PS8-76C4 (Harmarville) Resin†	79
	S-compounds	.05	Approx. 10 percent thiophenic sulfur-compounds		
	N-compounds	.10	Approx. 20 percent pyridines and quinolines		
	NS-compounds	.04	Mostly misidentified N-compounds		
	O-compounds	.22	Approx. 60 percent aliphatic and aromatic O-compounds ("Neutral" resin compounds)		
	O_2-compounds	.03			
	NO-compounds	.02	Mostly misidentified O-compounds		
	Hydrocarbons	.46	Few (if any) hydrocarbons present	API PS8-76D4 (Harmarville) Resin†	79
	S-compounds	.14	35-40 percent, mostly thioles, sulfides thiophenes(?) etc.		
	N-compounds	.11	Approx. 20 percent, aromatic types such as indoles, carbazoles		

(Continued)

Table 45 (Continued)

Material	Compound Type	Total Ion Fraction	Estimated Concentration	Sample Description/Source	Reference
Petroleum crude	NS-compounds	.07	Mostly misidentified N- and S-compound peaks	API PS8-76D4 (Harmarville) Resin[†]	79
	O-compounds	.12	20-30 percent aromatic and aliphatic O-compounds, e.g. phenols, acids, etc.		
	O_2-compounds	.02			
	NO-compounds	.08	15-20 percent aliphatic and aromatic amides, etc.		
	Hydrocarbons	.46	Approx. 5 percent aromatics	API PS8-76D5 (Harmarville) Resin[†]	79
	S-compounds	.07	Approx. 15 percent mostly polyaromatic thiophenes		
	N-compounds	.13	Approx. 20 percent 3-5 aromatic ring N-compounds (carbazole homologue)		
	NS-compounds	.09	Less than 15 percent, compound types uncertain, includes misidentified N- and S-compounds		
	O-compounds	.05	Less than 8 percent, peaks are mostly unresolved or misidentified NO-compounds or fragment ions from them		
	O_2-compounds	.02			

(Continued)

Table 45 (Concluded)

Material	Compound Type	Total Ion Fraction	Estimated Concentration	Sample Description/Source	Reference
Petroleum crude	NO-compounds	.17	Approx. 35-40 percent aromatic and aliphatic NO-compounds (e.g. amides etc.)		
	Hydrocarbons	.58	Up to 20 percent	API PS8-76C5 (Harmarville) Resin‡	79
	S-compounds	.04	Less than 8 percent polyaromatic thiophenes		
	N-compounds	.04	Poorly defined, inconclusive up to 15 percent NS compounds		
	NS-compounds	.07			
	O-compounds	.12	Approx. 30-35 percent aliphatic and aromatic O- and O_2-compounds		
	O_2-compounds	.05			
	NO-compounds	.10	Approx. 20-25 percent aromatic and aliphatic NO-compounds		
Raw shale oil	NA	NA	NA	--	--
Hydrotreated shale oil	NA	NA	NA	--	--

Explanatory Notes

*Data obtained under API Project PS-8-GST-(989-300)
†Data pertain to resin fractions of crudes obtained via SARA separation and boiling between 550-700°F.
‡Data pertain to resin fractions of crudes obtained via SARA separation and boiling between 700-1070°F.

Table 46. Distribution of Sulfur- and Oxygen-Containing Compound Classes by Mass Spectrometric Z Number

A. Monoaromatic Concentrates

Material	Mass Z Series	Prudhoe Bay 370-535°C monoaromatics, wt. %	Gach Saran 370-535°C monoaromatics, wt. %	Swan Hills 370-535°C monoaromatics, wt. %	Wilmington 370-535°C monoaromatics, wt. %	Recluse 370-530°C monoaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	0S	trace	0.61	ND	.10	.88	Alkylmonocyclic sulfides.	4
	-2S	ND	.14	ND	.04	.91	Alkylbicyclic sulfides.	
	-4S	ND	ND	ND	.06	.99	Alkyltricyclic sulfides.	
	-6S	ND	ND	ND	.04	.76	Alkyltetracyclic sulfides.	
	-8S	ND	ND	ND	.04	ND	Alkylpentacyclic sulfides	
	-10S	ND	ND	ND	.07	ND	Alkylhexacyclic sulfides.	
	-12S	ND	ND	ND	.14	ND	Alkylheptacyclic sulfides.	
	-4S	ND	ND	ND	.44	ND	Alkylthiophenes.	
	-6S	ND	ND	ND	.25	ND	Alkylnaphthenothiophenes.	
	-8S	ND	ND	ND	.41	ND	Alkyldinaphthenothiophenes.	
	-8S	.02	ND	ND	ND	ND	Naphthenophenylalkyl sulfides.	
	-14S	.05	ND	ND	ND	ND	Tetranaphthenophenylalkyl sulfides.	
	-16S	.01	ND	ND	ND	ND	Pentanaphthenophenylalkyl sulfides.	
	-10S	1.91	3.39	1.17	2.15	.64	Alkylbenzothiophenes.	
	-12S	.23	2.50	.88	1.52	.91	Alkylnaphthenobenzothiophenes.	
	-14S	.09	1.06	ND	1.22	ND	Alkyldinaphthenobenzothiophenes.	
	-16S	.08	ND	ND	.11	ND	Alkyltrinaphthenobenzothiophenes.	
	$-14S_2$	trace	.01	.01	.01	ND	Alkldiphenyldisulfides.	
	$-16S_2$	ND	ND	.01	ND	ND	Alkylnaphthenodiphenyldisulfides.	
	$-18S_2$	ND	ND	trace	ND	ND	Alkyldinaphthenodiphenyldisulfides.	
	$-20S_2$	ND	ND	trace	ND	ND	Alkytrinaphthenodiphenyldisulfides.	
	$-16S,-6S_2$	.10	1.35	.16	.28	ND	Alkylbenzopentacyclicdsulfides, alkylthienacyclic sulfides.	
	$-18S,-8S_2$	.16	1.68	.09	.55	ND	Alkylbenzohexacyclic sulfides, alkylthienobicyclic sulfides.	
	$-20S,-10S_2$	.08	.63	.05	.95	ND	Alkylbenzoheptacyclic sulfides, alkylthienotricyclic sulfides.	
	$-8S,-12S_2$	.08	ND	.03	.39	ND	Alkylbenzocyclic sulfides, alkylthienotetracyclic sulfides.	
	$-10S,-14S_2$	ND	ND	.03	.35	ND	Alkylbenzobicyclic sulfides, alkylthienopentacyclic sulfides.	
	$-12S,-16S_2$	ND	ND	.05	.14	ND	Alkylbenzotricyclic sulfides, alkylthienohexacyclic sulfides.	
	$-14S,-18S_2$	ND	ND	.05	.21	ND	Alkylbenzotetracyclic sulfides, alkylthienoheptacyclic sulfides.	
	$-16S,-20S_2,-10S_3$	ND	ND	.04	trace	ND	Alkyldibenzobicyclic sulfides, alkylbenzothienopentacyclic sulfides, alkyldithienocyclic sulfides.	
	$-18S,-22S_2,-12S_3$	ND	ND	.08	.04	ND	Alkyldibenzotricyclic sulfides, alkylbenzothienohexacyclic sulfides, alkyldithienobicyclic sulfides	

(Continued)

Table 46 (Continued)

A. Monoaromatic Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C monoaromatics, wt. %	Gach Saran 370-535°C monoaromatics, wt. %	Swan Hills 370-535°C monoaromatics, wt. %	Wilmington 370-535°C monoaromatics, wt. %	Recluse 370-530°C monoaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	$-20S,-24S_2,-14S_3$	ND	ND	.19	.08	ND	Alkyldibenzotetracyclic sulfides, alkylbenzothienoheptacyclic sulfides, alkyldithienatricyclic sulfides.	4
	$-22S,-12S_2,-16S_3$	ND	ND	.15	.12	ND	Alkyldibenzopentacyclic sulfides, alkylbenzothienocyclic sulfides, alkyldithienotetracyclic sulfides.	
	$-24S,-14S_2,-18S_3$	ND	ND	.08	.08	ND	Alkyldibenzohexacyclic sulfides, alkylbenzothienobicyclic sulfides, alkyldithienopentacyclic sulfides.	
	$-26S,-16S_2,-20S_3$	ND	ND	ND	.04	ND	Alkylidbenzaheptacyclic sulfides, Alkylbenzothienotricyclic sulfides, alkyldithienohexacyclic sulfides.	
	$-14S,-18S_2,22S_3$	.16	ND	ND	trace	ND	Alkyldibenzocyclic sulfides, alkylbenzothienotetracyclic sulfides, alkyldithienoheptacyclic sulfides.	
	-6(Nominal)	ND	ND	ND	.27	ND	Unknown	
	-10(Nominal)	ND	ND	ND	.71	ND	Unknown	
	OTHER	1.26	1.50	0.14	1.16	ND	--	
Raw shale oil				-NA-			--	--
Hydrotreated shale oil				-NA-			--	--

(Continued)

Table 46 (Continued)

A. Monoaromatic Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C monoaromatics, wt. %	Gach Saran 370-535°C monoaromatics, wt. %	Swan Hills 370-535°C monoaromatics, wt. %	Wilmington 370-535°C monoaromatics, wt. %	Recluse 370-530°C monoaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	$-20S,-24S_2,-14S_3$	ND	ND	.19	.08	ND	Alkyldibenzotetracyclic sulfides, alkylbenzothienoheptacyclic sulfides, alkyldithienatricyclic sulfides.	4
	$-22S,-12S_2,-16S_3$	ND	ND	.15	.12	ND	Alkyldibenzopentacyclic sulfides, alkylbenzothienocyclic sulfides, alkyldithienotetracyclic sulfides.	
	$-24S,-14S_2,-18S_3$	ND	ND	.08	.08	ND	Alkyldibenzohexacyclic sulfides, alkylbenzothienobicyclic sulfides, alkyldithienopentacyclic sulfides.	
	$-26S,-16S_2,-20S_3$	ND	ND	ND	.04	ND	Alkylidbenzaheptacyclic sulfides, Alkylbenzothienotricyclic sulfides, alkyldithienohexacyclic sulfides.	
	$-14S,-18S_2,22S_3$	.16	ND	ND	trace	ND	Alkyldibenzocyclic sulfides, alkylbenzothienotetracyclic sulfides, alkyldithienoheptacyclic sulfides.	
	-6(Nominal)	ND	ND	ND	.27	ND	Unknown	
	-10(Nominal)	ND	ND	ND	.71	ND	Unknown	
	OTHER	1.26	1.50	0.14	1.16	ND	--	
Raw shale oil				-NA-			--	--
Hydrotreated shale oil				-NA-			--	--

(Continued)

Table 46 (Continued)

B. Diaromatic Concentrates

Material	Mass Z Series	Prudhoe Bay 370-535°C diaromatics, wt. %	Gach Saran 370-535°C diaromatics, wt. %	Swan Hills 370-535°C diaromatics, wt. %	Wilmington 370-535°C diaromatics, wt. %	Recluse 370-530°C diaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	0S	ND	ND	ND	1.17	ND	Alkylmonocyclic sulfides.	4
	-2S	.11	ND	ND	1.29	ND	Alkylbicyclic sulfides.	
	-4S	.16	ND	ND	.91	ND	Alkyltricyclic sulfides.	
	-6S	.42	.24	ND	.42	ND	Alkyltetracyclic sulfides.	
	-8S	ND	.31	ND	.51	ND	Alkylpentacyclic sulfides	
	-10S	ND	ND	ND	1.05	ND	Alkylhexacyclic sulfides.	
	-12S	ND	ND	ND	1.20	ND	Alkylheptacyclic sulfides.	
	-14S	ND	ND	ND	.68	ND	Alkyloctocyclic sulfides.	
	-6S	ND	ND	ND	.60	ND	Alkylnaphthenothiphenes.	
	-8S	ND	ND	ND	.93	ND	Alkldinaphthenothiophenes.	
	-10S	4.32	9.45	1.95	3.44	ND	Alkylbenzothiophenes.	
	-12S	3.68	6.90	1.18	3.59	ND	Alklynaphthenobenzothiophenes.	
	-14S	2.53	5.75	.66	2.56	ND	Alkyldiaphthenobenzothiophenes.	
	-16S	7.19	8.47	.67	4.39	ND	Alkyltriaphthenobenzothiophenes and alkyldibenzothiophenes.	
	-18S	3.48	.50	.22	2.70	ND	Alklytetranaphthenobenzothiophenes and alkylnaphthenodibenzothiophenes.	
	-20S	.13	.10	ND	.51	ND	Alklpentanaphthenobenzothiophenes and/or alkyldinaphthenodibenzothiophenes.	
	-22S	.01	.06	ND	.98	ND	Alkylhexanaphthenobenzothiophenes and/or alkytrinaphthenodibenzothiophenes.	

(Continued)

Table 46 (Continued)

B. Diaromatic Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C diaromatics, wt. %	Gach Saran 370-535°C diaromatics, wt. %	Swan Hills 370-535°C diaromatics, wt. %	Wilmington 370-535°C diaromatics, wt. %	Recluse 370-530°C diaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	-24S	ND	ND	ND	trace	ND	Alkylheptanaphthenobenzothiophenes and/or alkyltetranaphthenodibenzothiophenes.	4
	-14S	ND	ND	ND	ND	.01	Alkylthienoindenes.	
	-16S	ND	ND	.14	ND	.20	Alkyldibenzothiophenes.	
	-18S	ND	ND	.17	ND	.30	Alkylnaphthenodibenzothiophenes.	
	-20S	ND	ND	.04	ND	.21	Alkyldinaphthenodibenzothiophenes.	
	-22S	ND	ND	.04	ND	.12	Alkyltrinaphthenodibenzothiohenes.	
	-24S	ND	ND	ND	ND	.07	Alkyltetranaphthenodibenzothiophenes.	
	-26S	ND	ND	ND	ND	.02	Alkylpentanaphthenodibenzothiophenes.	
	$-10S_2$	ND	ND	ND	ND	.03	Alkyldithienoindenes.	
	$-14S_2$	2.60	3.28	ND	2.87	ND	Alkyldiphenyldisulfides.	
	$-16S_2$	1.45	2.73	ND	3.65	ND	Alkylnaphthenodiphenyldisulfides.	
	$-18S_2$	.32	2.19	ND	1.61	ND	Alkyidinaphthenodiphenydisulfides.	
	$-20S_2$	ND	1.21	ND	ND	ND	Alkyltrinaphthenodiphenyldisulfides.	
	$-6S,-10S_2$	ND	ND	ND	ND	.95	Alkylphenyl sulfides, trinaphthenoalkylthienyl sulfides.	
	$-8S,-12S_2$	--	--	--		1.88	Naphthenoalkylinphenyl sulfides, tetrananphthenoalkylthienyl sulfides.	
	$-10S,14S_2$	--	--	--	--	.41	Dinaphthenoalkylphenyl sulfides, pentanaphthenoalkylthianyl sulfides.	

(Continued)

Table 46 (Continued)

B. Diaromatic Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C diaromatics, wt. %	Gach Saran 370-535°C diaromatics, wt. %	Swan Hills 370-535°C diaromatics, wt. %	Wilmington 370-535°C diaromatics, wt. %	Recluse 370-530°C diaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	$-16S,-6S_2$	ND	ND	.59	.03	ND	Alkylbenzopentacyclic sulfides, alkylthienacyclic sulfides.	4
	$-18S,-8S_2$	ND	ND	.28	.04	ND	Alkylbenzohexacyclic sulfides, alkylthienobicyclic sulfides.	
	$-20S,-10S_2$	ND	ND	.47	.05	ND	Alkylbenzoheptacyclic sulfides, alkythienotricyclic sulfides.	
	$-8S,-12S_2$	ND	ND	ND	.07	ND	Alkylbenzocyclic sulfides, alkylthienotetracyclic sulfides.	
	$-10S,-14S_2$	ND	ND	ND	.20	ND	Alkylbenzobicyclic sulfides, alkylthienopentacyclic sulfides.	
	$-12S,-16S_2$	ND	ND	ND	.03	ND	Alkylbenzatricyclic sulfides, alkylthienohexacyclic sulfides.	
	$-14S,-18S_2$	ND	ND	ND	.01	ND	Alkylbenzotetracyclic sulfides, alkylthienoheptacyclic sulfides.	
	$-16S,-20S_2,-10S_3$	ND	ND	ND	.04	ND	Alkyldibenzodicyclic sulfides, alkylbenzothienopentacyclic sulfides, alkyldithienocyclic sulfides.	
	$-18S,-22S_2,-12S_3$	ND	ND	ND	.04	ND	Alkyldibenzatricyclic sulfides, alkylbenzothienohexacyclic sulfides, alkyldithienobicyclic sulfides.	

(Continued)

Table 46 (Continued)

B. Diaromatic Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C diaromatics, wt. %	Gach Saran 370-535°C diaromatics, wt. %	Swan Hills 370-535°C diaromatics, wt. %	Wilmington 370-535°C diaromatics, wt. %	Recluse 370-530°C diaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	$-20S,-24S_2,-14S_2$	ND	ND	ND	.03	ND	Alkyldibenzotetracyclic sulfides, alkylbenzothienoheptacyclic sulfides, alkyldithienotricyclic sulfides.	4
	$-22S,-12S_2,-16S_3$	ND	ND	ND	.04	ND	Alkyldibenzopentacyclic sulfides, alkylbenzothienocyclic sulfides, alkyldithienotetracyclic sulfides.	
	$-24S,-14S_2,-18S_3$	ND	ND	ND	.02	ND	Alkyldibenzohexacyclic sulfides, alkylbenzothienobicyclic sulfides, alkyldithienopentacyclic sulfides.	
	$-26S,-16S_2,-20S_3$	ND	ND	ND	.04	ND	Alkyldibenzoheptacyclic sulfides, alkylbenzothienotricyclic sulfides, alkyldithienohexacyclic sulfides.	
	$-14S,-18S_2,-22S_3$	ND	ND	ND	.03	ND	Alkyldibenzocyclic sulfides, alkylbenzothienotetracyclic sulfides, alkyldithienoheptacyclic sulfides.	
	-6(Nominal	ND	ND	.01	.06	ND	Unknown.	
	-8(Nominal)	ND	ND	.01	ND	ND	Unknown	
	-10(Nominal)	.07	.10	.01	ND	ND	Unknown	
	-12(Nominal)	ND	ND	ND	.07	ND	Unknown	
	-14(Nominal)	ND	ND	ND	.08	ND	Unknown	

(Continued)

Table 46 (Continued)

B. Diaromatic Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C diaromatics, wt. %	Gach Saran 370-535°C diaromatics, wt. %	Swan Hills 370-535°C diaromatics, wt. %	Wilmington 370-535°C diaromatics, wt. %	Recluse 370-530°C diaromatics, wt. %	Probable Compound Type	Reference
Petroleum crude	-16(Nominal)	ND	ND	ND	.04	ND	Unknown.	4
	-18(nominal)	ND	ND	ND	.05	ND	Unknown.	
	OTHER	1.85	2.62	1.27	0.75	ND	--	
Raw shale oil				-NA-			--	--
Hydrotreated shale oil				-NA-			--	--

C. Polyaromatic - Polar Concentrates

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude								
	0S	1.42	6.40	.47	3.45	ND	Alkylcyclic sulfides	4
	-2S	4.10	7.50	.99	5.35	ND	Alkylbicyclic sulfides.	
	-4S	5.16	7.38	1.24	6.00	ND	Alkyltricyclic sulfides.	
	-6S	4.18	6.92	1.27	4.40	ND	Alkyltetracyclic sulfides.	
	-8S	3.31	7.00	.84	4.46	ND	Alkylpentacyclic sulfides.	
	-10S	1.79	5.46	1.37	3.73	ND	Alkylhexacyclic sulfides.	
	-12S	1.41	7.07	trace	3.35	ND	Alkylheptacyclic sulfides.	
	-22	1.57	.04	.44	.15	.19	Alkylpyrenes.	
	-24	.58	.03	.28	.06	ND	Alkylnaphthenopyrenes.	
	-26	.37	.53	.06	ND	ND	Alkyldinaphthenopyrenes.	
	-28	ND	.35	ND	ND	ND	Alkytrinaphthenopyrenes.	
	-24	.58	ND	.27	ND	.21	Alkylbenzophenanthrenes/anthracenes.	
	-26	ND	.53	.05	.07	ND	Alkylnaphthenobenzophenathrenes/ anthracenes.	
	-28	ND	.35	ND	ND	ND	Alkyldinaphthenobenzophenanthrenes/ anthracenes.	

(Continued)

Table 46 (Continued)

C. Polyaromatic - Polar Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude	-28	ND	.35	ND	ND	ND	Alkyldinaphthenobenzophenanthrenes/ anthracenes.	4
	-28	ND	.01	.38	.14	.46	Alkylbenzopyrenes/perylenes.	
	-30	ND	ND	ND	.04	ND	Alkylnaphthenobenzopyrenes/ perylenes.	
	-16S	2.05	4.35	.65	4.07	.37	Alkyldibenzothiophenes/ naphthothiophenes.	
	-18S	2.02	2.80	1.60	3.42	.47	Alkylnaphthenodibenzathiophenes/ naphthothiophenes.	
	-20S	1.76	2.49	.69	2.01	.45	Alkyldinaphthenodibenzathiophenes/ naphthothiophenes.	
	-22S	1.83	3.68	ND	.87	1.21	Alkyltrinaphthenodibenzothiophenes/ naphthothiophenes.	
	-24S	.58	1.56	ND	.65	.47	Alkyltetranaphthenodibenzothiophenes/ naphthothiophenes.	
	-26S	.40	1.19	ND	ND	.45	Alkylpentanaphthenodibenzathiophenes/ naphthothiophenes.	
	-28S	.26	.85	ND	ND	.54	Alkylhexanaphthenodibenzothiophenes/ naphthothiophenes.	
	-22S	1.84	ND	ND	.70	ND	Alkylthienophenanthrenes/anthracenes.	
	-24S	.58	ND	ND	.38	ND	Alkyldinaphthenothienophenanthracenes/ anthracenes and/or alkylthienodiacenapthalenes.	

(Continued)

Table 46 (Continued)

C. Polyaromatic - Polar Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude	-26S	.40	ND	ND	.28	ND	Alkyldinaphthenothienophenanthracenes/anthracenes and/or alkylnaphthenothienodiacenaphthalenes.	4
	-28S	.27	ND	ND	.10	ND	Alkyltrinaphthenothienophenanthrenes/anthracenes and/or alkyldinaphthenothienodiacenaphthalenes.	
	-30S	ND	ND	ND	.03	ND	Alkyltetranaphthenothienophenanthrenes/anthracenes.	
	-32S	ND	ND	ND	.05	ND	Alkylpentanaphthenothienophenanthrenes/anthracenes.	
	-20S	ND	ND	.69	.93	.27	Alkylthienobenzoindenes.	
	-22S	ND	ND	2.03	.70	ND	Alkylnaphthenothienobenzoindenes.	
	-24S	ND	ND	1.32	.38	ND	Alkyldinaphthenothienobenzoindenes.	
	-26S	ND	ND	.53	.28	ND	Alkyltrinaphthenothienobenzoindenes.	
	-28S	ND	ND	.71	.10	ND	Alkyltetranaphthenothienobenzoindenes.	
	-30S	ND	ND	ND	.03	ND	Alkylpentanaphthenothienobenzoindenes.	
	-32S	ND	ND	ND	.05	ND	Alkylhexanaphthenothienobenzoindenes.	
	-14S	ND	.34	ND	ND	ND	Alkylthienoindenes.	
	-26S	ND	ND	ND	.07	.02	Alkylthienopyrenes.	
	-28S	ND	ND	ND	.02	ND	Alkylnaphthenothienopyrenes.	
	-28S	ND	ND	ND	ND	.01	Alkylthienobenzophenanthrenes/anthracenes.	

(Continued)

Table 46 (Continued)

C. Polyaromatic - Polar Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude	-30S	.04	ND	.03	ND	ND	Alkylnaphthenothienobenzophenanthrenes/anthracenes.	4
	-32S	.06	ND	.01	.06	ND	Alkythienobenzapyrenes/perylenes.	
	-34S	ND	ND	ND	.03	ND	Alkylthienodibenzophenanthrenes/anthracenes.	
	$-14S_2$	ND	ND	ND	2.97	ND	Alkyldiphenyldisulfides.	
	$-16S_2$	ND	ND	ND	1.85	ND	Alkylnaphthenodiphenyldisulfides.	
	$-18S_2$	ND	ND	ND	.87	ND	Alkyldinaphthenodiphenyldisulfides.	
	$-20S_2$	1.04	1.11	.93	.43	.96	Alkylthienodibenzothiophenes/naphthothiophenes.	
	$-22S_2$	.58	.79	1.85	.30	1.07	Alkylnaphthenothienodibenzothiophenes/naphthothiophenes.	
	$-24S_2$	.24	.41	.94	.03	.81	Alkyldinaphthenothienodibenzothiophenes/naphthothiophenes.	
	$-26S_2$	.21	ND	ND	.03	.51	Alklytrinaphthenothienodibenzothiophenes/naphthothiophenes.	
	$-28S_2$	.08	ND	ND	ND	.29	Alkyltetranaphthenothienodibenzothiophenes/naphthothiaphenes.	
	$-26S_2$	ND	.50	.22	ND	ND	Alkyldithienophenanthrenes/anthracenes.	

(Continued)

Table 46 (Continued)

C. Polyaromatic - Polar Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude	$-28S_2$	ND	.17	ND	ND	ND	Alkylnaphthenodithienophenathrenes/ anthracenes and/or alkyldithienodiacenaphthalenes.	4
	$-30S_2$	.04	.09	ND	ND	ND	Alkyldinaphthenodithienophenanthrenes/ anthracenes and/or alkylnaphthenodithienodiacenaphthalenes.	
	$-32S_2$	ND	.03	ND	ND	ND	Alkyltrinaphthenodithienophenanthrenes/ anthracenes and/or alkyldinaphthenodithienodiacenaphthalenes.	
	$-24S_2$	ND	ND	.63	.24	ND	Alkyldithienobenzoindenes.	
	$-26S_2$	ND	ND	.47	.45	ND	Alkylnaphthenodithienobenzoindenes.	
	$-28S_2$	ND	ND	.91	ND	ND	Alkyldinaphthenodithienobenzoindenes.	
	$-30S_2$	ND	ND	.19	ND	ND	Alkyltrinaphthenodithienobenzoindenes.	
	$-32S_2$	ND	ND	.06	ND	ND	Alkyltetranaphthenodithienobenzoindenes.	
	$-32S_2$	ND	ND	ND	.02	ND	Alkyldithienobenzophenanthrenes/ anthracenes.	
	$-24S_3$	.10	.49	.12	ND	ND	Alkyldithienodibenzothiophenes/ naphthothiophenes.	
	$-26S_3$	.04	.13	.15	ND	ND	Alkylnaphthenodithienodibenzothiophenes/ naphthothiophenes.	
	$-28S_3$	ND	.09	ND	ND	ND	Alkyldinaphthenodithienodibenzothiophenes/ naphthothiophenes.	

(Continued)

Table 46 (Continued)

C. Polyaromatic - Polar Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude	$-28S_3$	ND	ND	.07	ND	ND	Alkyltrithienobenzoindenes.	4
	$-30S_3$	NDZ	ND	ND	.02	ND	Alkylnaphthenotrithienobenzoindenes.	
	$-6S_2,-16S$	.61	ND	ND	.16	.22	Alkylthienocylcic sulfides, alkylbenzopentacyclic sulfides.	
	$-8S_2,-18S$	.69	ND	ND	.16	.24	Alkylthienobicyclic sulfides, alkylbenzohexacyclic sulfides.	
	$-10S_2,-20S$	.50	ND	ND	.08	.20	Alkylthienotricyclic sulfides, alkylbenzoheptacyclic sulfides.	
	$-12S_2,-8S$	.72	ND	ND	.34	.66	Alkylthienotetracyclic sulfides, alkylbenzocyclic sulfides.	
	$-14S_2,-10S$	.72	ND	ND	.07	1.22	Alkylthienopentacyclic sulfides, alkylbenzobicyclic sulfides.	
	$-16S_2,-12S$	ND	ND	ND	.07	ND	Alkylthienohexacyclic sulfides, alkylbenzotricyclic sulfides.	
	$-18S_2,-14S$	ND	ND	ND	.13	ND	Alkylthienoheptacyclic sulfides, alkylbenzotetracyclic sulfices.	
	$-10S_3,-20S_2,-16S$	.02	.04	.01	.18	.02	Alkyldithienocyclic sulfides, alkylbenzothienopentacyclic sulfides, alkyldibenzobicyclic sulfides.	

(Continued)

Table 46 (Concluded)

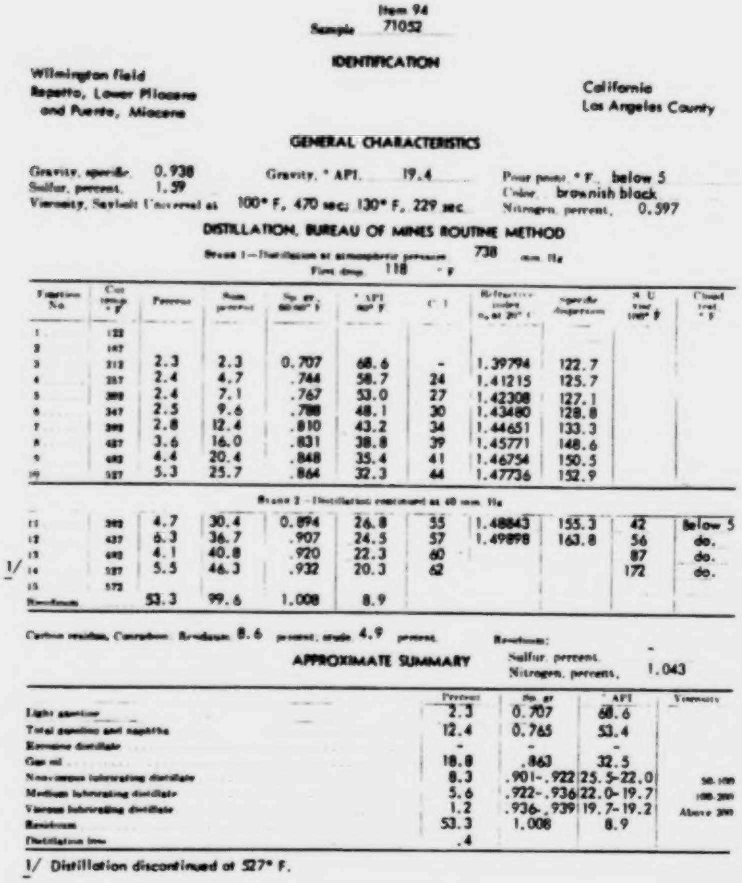
C. Polyaromatic - Polar Concentrates (Continued)

Material	Mass Z Series	Prudhoe Bay 370-535°C Polyaromatic, polar	Gach Saran 370-535°C Polyaromatic, polar	Swan Hills 370-535°C Polyaromatic, polar	Wilmington 370-535°C Polyaromatic, polar	Recluse 370-530°C Polyaromatic, polar	Probable Compound Type	Reference
Petroleum crude	$-12S_3,-22S_2,-18S$	ND	.10	.02	.17	.02	Alkyldithienobicyclic sulfides, alkylbenzothienohexacyclic sulfides, alkyldibenzotricyclic sulfides.	4
	$-14S_3,-24S_2,-20S$	.01	.41	.02	.10	.01	Alkyldithienotricyclic sulfides, alkylbenzothienoheptacyclic sulfides, alkyldibenzotetracyclic sulfides.	
	$-16S_3,-12S_2,-22S$	ND	.50	.05	.12	05	Alkyldithienotetracyclic sulfides, alkylbenzothienocyclic sulfides, alkyldibenzopentacyclic sulfides.	
	$-18S_3,-14S_2,-24S$	ND	.17	.02	.08	.01	Alkyldithienopentacyclic sulfides, alkylbenzothienobicyclic sulfides, alkylbenzoheptacyclic sulfides.	
	$-20S_3,-16S_2,-26S$	ND	.09	.04	.07	ND	Alkyldithienohexacyclic sulfides, Alkylbenzothienotricyclic sulfides, alkyldibenzoheptacyclic sulfices.	
	$-22S_3,-18S_2,-14S$	ND	.07	.03	.13	.01	Alkyldithienoheptacyclic sulfides, alkylbenzothienotetracyclic sulfides, alkyldibenzocyclic sulfides.	
	-26(Nominal)	.43	ND	.03	ND	ND	Unknown	
	-20(Nominal)	ND	ND	ND	.05	ND	Unknown.	
	-22(Nominal)	ND	.01	ND	.04	ND	Unknown.	
	-28(Nominal)	ND	ND	ND	.20	ND	Unknown.	
	-18(Nominal)	ND	.26	ND	ND	ND	Unknown.	
	-24(Nominal)	1.14	ND	ND	ND	ND	Unknown.	
	OTHER	2.60	6.71	1.36	3.53	0.01		
Raw shale oil				-NA-			--	--
Hydrotreated shale oil				-NA-			--	--

Explanatory Note

*Details of the sample preparation and analysis procedures (which include GPC, NMR and MS techniques) are provided in Reference 4 (see Table 37).

Table 47. Typical BETC Crude Oil Analysis (Wilmington, CA High Sulfur Crude) (3)



Item 94
Sample 71052

IDENTIFICATION

Wilmington field
Repetto, Lower Pliocene
and Puente, Miocene

California
Los Angeles County

GENERAL CHARACTERISTICS

Gravity, specific 0.938
Sulfur, percent, 1.59
Viscosity, Saybolt Universal at 100° F, 470 sec; 130° F, 229 sec
Gravity, °API 19.4
Pour point, °F, below 5
Color, brownish black
Nitrogen, percent, 0.597

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Stage 1—Distillation at atmospheric pressure 738 mm. Hg
First drop 118 °F

Fraction No.	Cut temp. °F	Percent	Sum percent	Sp. gr., 60/60° F	°API 60° F	C. I.	Refractive index n_D at 20° C	Specific dispersion	S. U. visc. 100° F	Cloud test °F
1	122									
2	167									
3	212	2.3	2.3	0.707	68.6	-	1.39794	122.7		
4	257	2.4	4.7	.744	58.7	24	1.41215	125.7		
5	302	2.4	7.1	.767	53.0	27	1.42308	127.1		
6	347	2.5	9.6	.788	48.1	30	1.43480	128.8		
7	392	2.8	12.4	.810	43.2	34	1.44651	133.3		
8	437	3.6	16.0	.831	38.8	39	1.45771	148.6		
9	482	4.4	20.4	.848	35.4	41	1.46754	150.5		
10	527	5.3	25.7	.864	32.3	44	1.47736	152.9		

Stage 2—Distillation continued at 40 mm. Hg

Fraction No.	Cut temp. °F	Percent	Sum percent	Sp. gr., 60/60° F	°API 60° F	C. I.	Refractive index n_D at 20° C	Specific dispersion	S. U. visc. 100° F	Cloud test °F
11	392	4.7	30.4	0.894	26.8	55	1.48843	155.3	42	below 5
12	437	6.3	36.7	.907	24.5	57	1.49898	163.8	56	do.
13	482	4.1	40.8	.920	22.3	60			87	do.
1/ 14	527	5.5	46.3	.932	20.3	62			172	do.
15	572									
Residuum		53.3	99.6	1.008	8.9					

Carbon residue, Conradson: Residuum 8.6 percent; crude 4.9 percent.

Residuum:
Sulfur, percent, -
Nitrogen, percent, 1.043

APPROXIMATE SUMMARY

	Percent	Sp. gr.	°API	Viscosity
Light gasoline	2.3	0.707	68.6	
Total gasoline and naphtha	12.4	0.765	53.4	
Kerosine distillate	-	-	-	
Gas oil	18.8	.863	32.5	
Nonviscous lubricating distillate	8.3	.901-.922	25.5-22.0	50-100
Medium lubricating distillate	5.6	.922-.936	22.0-19.7	100-200
Viscous lubricating distillate	1.2	.936-.939	19.7-19.2	Above 200
Residuum	53.3	1.008	8.9	
Distillation loss	.4			

1/ Distillation discontinued at 527° F.

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Table 48. Typical BETC Crude Oil Analysis
(Castaic Junction, CA High Nitrogen Crude) (1)

CRUDE PETROLEUM ANALYSIS

Bureau of Mines Bartlesville Laboratory
Sample 55125

IDENTIFICATION

Castaic Junction field	California
Mohnian-Miocene Zone 10 sand	Los Angeles County
10,640-10,790 feet	4N-17W

GENERAL CHARACTERISTICS

Specific gravity, 0.940
A. P. I. gravity, 19.0°
Pour point, °F., 10
Sulfur, percent 3.40
Color, brownish black
Saybolt Universal viscosity at 100° F., 1,230 sec.; at 130° F., 620 sec.
Nitrogen, percent, 0.871

DISTILLATION, BUREAU OF MINES ROUTINE METHOD

Stage 1—Distillation at atmospheric pressure, 747 mm. Hg
First drop, 30 ° C. (86 ° F.)

Fraction No.	Cut temp. °F.	Percent	Sum, percent	Sp. gr., 60/60° F.	°A. P. I., 60° F.	C. I.	Refractive index N_D at 20° C.	Specific dispersion	S. U. visc., 100° F.	Cloud test, °F.
1	122	1.6	1.6	0.654	84.9	-				
2	167	1.4	3.0	.681	76.3	13				
3	212	2.3	5.3	.723	64.2	23	1.38771	123.8		
4	257	3.3	8.6	.747	57.9	25	1.41300	128.1		
5	302	3.3	11.9	.769	52.5	28	1.42458	130.6		
6	347	2.8	14.7	.788	48.1	30	1.43525	132.5		
7	392	2.4	17.1	.810	43.2	34	1.44654	136.1		
8	437	2.8	19.9	.829	39.2	38	1.45638	141.3		
9	482	3.8	23.7	.847	35.6	41	1.46643	147.8		
1/ 10	527	4.0	27.7	.860	33.0	-	1.47581	157.6		
Stage 2—Distillation continued at 40 mm. Hg										
11	392	2.9	30.6	0.878	29.7	-	1.48395	150.9	41	10
12	437	3.8	34.4	.886	28.2	47	1.48868	157.4	48	30
13	482	3.6	38.0	.905	24.9	53	-	-	63	45
14	527	5.6	43.6	.918	22.6	56	-	-	115	60
2/ 15	572	2.6	46.2	.934	20.0	-	-	-	180	85
Residuum	.....	53.3	99.5	1.032	5.6					

Ramsbottom carbon residue: Residuum, 7.3 percent; crude, 4.3 percent.
Equivalent Conradson carbon residue: Residuum, 9.4 percent.

APPROXIMATE SUMMARY

	Percent	Sp. gr.	°A. P. I.	Viscosity
Light gasoline	5.3	0.691	73.3	
Total gasoline and naphtha	17.1	0.749	57.4	
Kerosine distillate	-	-	-	
Gas oil	16.0	.859	33.2	
Nonviscous lubricating distillate	6.4	.888-.914	27.9-23.3	50-100
Medium lubricating distillate	6.7	.914-.939	23.3-19.2	100-200
Viscous lubricating distillate	-	-	-	Above 200
Residuum	53.3	1.032	5.6	
Distillation loss	.5			

1/ Distillation discontinued at 509° F.
2/ Distillation discontinued at 545° F.

Table 49. Properties of Various Distillation Fractions of Paraho - SOHIO Toledo Refined Shale Oil (Reference 36)

A. Naphtha Fraction

Cut	165-220°F	220-280°F	280-340°F	340-380°F
Cum. Mid. Vol. %	0.04	1.25	4.48	8.36
Vol. % of Crude	0.07	2.35	4.11	3.65
Cum. Vol. % of Crude	0.07	2.42	6.53	10.18
Gravity, °API	60.0	58.3	52.4	48.0
Specific Gravity @ 60°F	0.7389	0.7455	0.7694	0.7883
Distillation, D-86				
IBP	Ins. Samp.	213	252	326
10% Rec.		230	279	342
30% Rec.		238	287	350
50% Rec.		247	297	353
70% Rec		255	306	360
90% Rec		271	318	369
EP		296	323	398
% Rec.		99.0	99.0	99.0
% Res.		1.0	1.0	1.0
UPO "K" Factor	NA	11.95	11.85	11.84
Elemental Analysis				
C, wt. %	85.00	85.26	85.18	85.52
H, wt. %	14.48	14.43	14.06	13.86
O, wt. %	0.84	0.59	0.50	0.58
N, wt. %	< 0.05	< 0.05	0.14	0.27
S, wt. %	0.068	0.008	0.002	< 0.002
Mercaptan S, ppm	Ins. Samp.	0	0	0
Pour Point, °F	NA	NA	NA	<-40
Freezing Point, °F	NA	NA	NA	-80.5
Aniline Point, °F	Ins. Samp.	128.0	128.5	131.5
Cetane Index	NA	NA	NA	46.1
Diesel Index	Ins. Samp.	74.5	67.3	63.0
Total Acid No., mgKOH/g	NA	NA	0.046	0.052
RI @140°F	NA	NA	1.4114	1.4220
Viscosity cs/100°F	NA	NA	0.85	1.06
Viscosity SSU/100°F	NA	NA	28.6	29.3
Viscosity cs/210°F	NA	NA	0.65	0.60
Viscosity SSU/210°F	NA	NA	28.0	27.9
PNA by MS, Vol. %				
Paraffins	45.14	49.25	40.51	0.00
Naphthenes	33.63	35.43	39.62	82.34
Aromatics	21.23	15.32	19.87	17.66

(Continued)

Table 49 (Continued)

B. Kerosene Fraction

Cut	380-480°F	480-520°F
Cum. Mid. Vol. %	17.10	26.49
Vol. % of Crude	13.83	4.96
Cum. Vol. % of Crude	24.01	28.97
Gravity, °API	40.6	36.3
Specific Gravity @ 60°F	0.8222	0.8433
Distillation, D-86		
IBP	384	446
10% Rec.	401	483
30% Rec.	410	488
50% Rec.	419	492
70% Rec.	429	496
90% Rec.	443	503
EP	461	511
% Rec.	99.0	99.0
% Res.	1.0	1.0
UOP "K" Factor	11.65	11.67
Elemental Analysis		
C, wt. %	86.03	86.08
H, wt. %	13.29	12.99
O, wt. %	0.66	0.95
N, wt. %	0.30	0.41
S, wt. %	< 0.002	< 0.002
Mercaptan S, ppm	0	0.98
Metals, ppm		
As	< 0.2	< 0.2
Na	< 0.1	< 0.1
K	< 0.5	< 0.5
V	< 0.006	< 0.006
Ni	< 0.02	< 0.02
Fe	0.04	0.13
Pour Point, °F	-40	-35
Freezing Point, °F	-47.2	-32.8
Cetane Index	42.8	48.5
Aniline Point, °F	130.5	135.5
Smoke Point, mm	24	24
Total Acid No., mgKOH/g	0.077	0.105
RI @140°F	1.4351	1.4527
Flash Point, °F	176	230
Ramsbottom Carbon, wt. %	0.143	0.207
Viscosity cs/100°F	1.63	2.52
Viscosity SSU/100°F	31.3	34.4
Viscosity cs/210°F	0.81	1.10
Viscosity SSU/210°F	28.6	29.7
PNA by MS, Vol. %		
Paraffins	36.01	38.65
Naphthenes	40.15	35.17
Aromatics	23.84	26.18

(Continued)

Table 49 (Continued)

C. Middle Distillate Fraction

Cut	520-600°F	600-650°F	650°-700°F
Cum. Mid. Vol. %	35.21	46.86	56.77
Vol. % of Crude	12.48	10.82	8.99
Cum. Vol. % of Crude	41.45	52.27	61.26
Gravity, °API	34.6	31.7	30.1
Specific Gravity @ 60°F	0.8519	0.8670	0.8756
Distillation, D-86			
IBP	492	581	618
10% Rec.	523	596	636
30% Rec.	527	598	638
50% Rec.	532	603	643
70% Rec.	540	608	645
90% Rec.	551	616	652
EP	564	626	662
% Rec.	99.0	99.0	99.0
% Res.	1.0	1.0	1.0
UPO "K" Factor	11.71	11.77	11.80
Elemental Analysis			
C, wt. %	86.40	86.91	86.52
H, wt. %	12.94	12.88	12.66
O, wt. %	1.13	0.59	0.17
N, wt. %	0.46	0.42	0.43
S, wt. %	<0.002	<0.002	<0.002
Mercaptan S, ppm	9.2	1.7	7.5
Metals, ppm			
As	<0.2	<0.2	<0.2
Na	<0.1	<0.1	<0.1
K	<0.5	<0.5	<0.5
V	<0.006	<0.006	<0.006
Ni	<0.02	<0.02	<0.02
Fe	0.06	0.08	0.09
Pour Point, °F	+5	+30	+55
Aniline Point, °F	145.0	155.5	165.0
Cetane Index	51.1	54.0	56.2
Total Acid No., mgKOH/g	0.085	0.052	0.042
RI @140°F	1.4596	1.4689	1.4729
Flash Point, °F	320	320	360
Ramsbottom Carbon, wt. %	0.052	0.029	0.046
Viscosity cs/100°F	4.04	6.68	10.47
Viscosity SSU/100°F	39.3	47.8	60.4
Viscosity cs/210°F	0.91	2.01	2.57
Viscosity SSU/210°F	29.0	32.9	34.8
PNA by MS, Vol. %			
Paraffins	30.42	17.72	NA
Naphthenes	19.18	12.98	NA
Aromatics	50.40	69.30	NA

(Continued)

Table 49 (Continued)

D. Heavy Distillate Fraction

Cut	700-750°F	750-800°F	800°-850°F	850-900°F	900-950°F	950-1000°F
Cum. Mid. Vol. %	66.04	75.35	82.63	87.88	91.57	94.24
Vol. % of Crude	9.56	9.06	5.49	5.01	2.38	2.96
Cum. Vol. % of Crude	70.82	79.88	85.37	90.38	92.76	95.72
Gravity, °API	29.5	29.0	28.3	27.1	27.8	30.1
Specific Gravity @ 60°F	0.8789	0.8816	0.8855	0.8922	0.8883	0.8756
Distillation, D-1160						
IBP	554	560	716	721	Ins. Samp	848
10% Rec.	718	746	793	848		901
30% Rec.	722	761	812	854		913
50% Rec.	727	767	820	856		926
70% Rec.	731	795	824	864		934
90% Rec.	742	791*	837	882		964
EP	750	799	854	916		982
% Rec.	99.0	99.0	99.0	98.0		98.0
% Res.	1.0	1.0	1.0	2.0		2.0
UPO "K" Factor	12.05	12.14	12.26	12.28	NA	12.73
Elemental Analysis						
C, wt. %	86.75	86.70	86.71	86.80	86.52	86.49
H, wt. %	12.61	12.77	12.91	12.86	13.09	13.22
O, wt. %	0.62	1.76	0.45	0.46	0.44	0.49
N, wt. %	0.41	0.28	0.20	0.16	0.13	0.14
S, wt. %	<0.002	<0.002	0.16	0.005	0.005	0.006
Mercaptan S, ppm	3.7	6.0	NA	NA	NA	NA
Metals, ppm						
As	<0.2	<0.2	0.1	0.2	0.1	0.2
Na	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
K	<0.5	<0.5	<0.4	0.5	<0.4	1.1
V	<0.006	<0.006	<0.005	<0.005	0.006	0.007
Ni	<0.02	0.04	0.06	0.02	0.01	0.02
Fe	0.08	0.09	0.4	<0.02	<0.2	0.3
Pour Point, °F	+70	+70	+110	+110	+115	+110
Aniline Point, °F	176.5	195.0	228.0	215.5	226.0	235.0
Total Acid No., mgKOH/g	0.031	0.036	0.147	0.117	0.129	0.102
RI @140°F	1.4792	1.4759	1.4767	Too dark	Too dark	Too dark
Flash Point, °F	395	430	465	490	505	540
C_5 Insols, wt. %	Nil	Nil	0.043	0.129	0.079	0.172
Ramsbottom Carbon, wt. %	0.051	0.062	0.104	0.087	0.095	0.128
Viscosity cs/100°F	16.18	25.71	NA	NA	NA	NA
Viscosity SSU/100°F	82.1	122.4	NA	NA	NA	NA
Viscosity cs/140°F	NA	NA	NA	23.43	23.03	27.13
Viscosity SSU/140°F	NA	NA	NA	112.7	111.0	129.0
Viscosity cs/210°F	3.27	4.53	5.85	7.65	7.97	9.04
Viscosity cs/210°F	37.1	41.2	45.4	51.2	52.3	55.9

(Continued)

Table 49 (Concluded)

E. Residue

Cut	800°F+	900°F+	1000°F+
Vol. % of Crude	20.12	9.62	4.28
Gravity, °API	28.4	29.5	29.4
Specific Gravity @ 60°F	0.8849	0.8789	0.8794
Distillation, D-11160			
IBP	772	854	916
10% Rec.	849	908	959
30% Rec.	859	916	974
50% Rec.	879	936	989
70% Rec.	918	979	1019
90% Rec.	999	NA	NA
EP	1007	1005	1055
% Rec.	93.0	84.0	86.0
% Res.	7.0	16.0	14.0
Elemental Analysis			
C, wt. %	86.55	86.52	86.52
H, wt. %	13.02	13.20	13.20
O, wt. %	0.56	0.71	0.72
N, wt. %	0.16	0.15	0.17
S, wt. %	0.011	0.008	0.013
Metals, ppm			
As	0.3	0.3	0.7
Na	<0.1	<0.1	<0.1
K	<0.4	0.6	<0.4
V	0.016	0.032	0.057
Ni	0.13	0.24	0.49
Fe	0.3	0.4	1.0
C_5 Insols, wt. %	0.277	0.729	1.560
Ramsbottom Carbon, wt. %	0.331	0.679	1.450
Viscosity cs/140°F	24.94	49.20	Too Heavy
Viscosity cs/210°F	8.43	11.08	15.67
Viscosity SSU/210°F	53.8	63.1	80.6

(Continued)

Table 50. Properties of Various Distillation Fractions of In-Situ, Rock Springs, WY Raw Shale Oil (Reference 81)

Cut	Dry Shale Oil	Naphtha	Light Distillate	Heavy Distillate	Residue
Boiling Range	NA	IBP - 400°F	400-600°F	600-800°F	≥800°F
Fraction Yield (vol. %)	NA	12.2	39.8	31.7	12.6
Alkanes and cycloalkanes (vol %)	NA	65.2	60.5	NA	NA
Olefins and cyclo-olefins (vol %)	NA	11.1	11.1	NA	NA
Aromatics (vol %) (includes sulfur, nitrogen and oxygen compounds)	NA	23.7	28.4	NA	NA
Carbon (wt %)	85.0	84.7	85.4	85.1	82.8
Hydrogen (wt %)	12.0	12.9	12.4	11.9	10.6
Nitrogen (wt %)	1.50	1.04	1.16	1.59	2.20
Sulfur (wt %)	0.95	0.69	0.44	0.52	0.94
Oxygen (wt %)	0.6	0.6	0.6	0.9	3.5
VPO Molecular Weight (av)	NA	199	204	290	NA
Tar Acids (vol %)	NA	3.6	1.6	NA	NA
Tar Bases (vol %)	NA	6.6	9.9	NA	NA

Table 51. Nitrogen, Sulfur and Oxygen Content in Various Distillation Fractions of API Crude Oils C and D (Reference 58)

Material	Value (wt %)	120-350°F	350-550°F	550-700°F	700-1070°F
API Crude Oil C	Nitrogen	0.0001	0.00075	0.0067	0.072
	Sulfur	0.014	0.077	0.18	0.47
	Oxygen	<0.01	0.03	0.18	0.27
API Crude Oil D	Nitrogen	0.0001	0.00032	0.0132	0.11
	Sulfur	0.026	0.41	1.87	2.98
	Oxygen	<0.01	0.055	<0.01	0.22

Table 52. Sulfur Content in Various Distillation Fractions of Petroleum Crudes (Wt. %)

Fraction	Cut Point (°F)	Wilmington, CA Crude (Ref. 4)	Recluse, WY Crude (Ref. 4)	Prudhoe Bay, AK Crude (Ref. 5)
1	122	ND	ND	ND
2	167	ND	ND	0.10
3	212	0.11	ND	0.01
4	257	0.03	ND	0.01
5	302	0.06	ND	0.01
6	347	0.14	ND	0.02
7	392	0.16	ND	0.03
8	437	0.23	ND	0.07
9	482	0.40	0.006	0.13
10	527	0.65	0.015	0.23
11	587	0.94	0.026	0.27
12	637	1.23	0.042	0.54
13	687	1.43	0.079	0.78
14	737	1.50	0.108	0.97
15	787	2.07	0.111	1.06
Residue	ND	1.59	0.193	1.86

Table 53. Hydrocarbon Compound Classes and Sulfur-Containing Compounds in Various Distillation Distillation Fractions of Alaskan North Slope Crude (Reference 6)

	Vol. %							Wt. %	Wt %
Cut Temperature, °F	55-165*	165-220	220-280	280-340	340-380	380-480	480-520	520-600	600-700
Paraffins	67.98	46.26	40.37	43.79	42.67	34.56	26.84	34.5	16.2
Cycloparaffins									
1 Ring	25.78	41.17	39.48	28.71	30.31	22.36	2480	14.8	13.7
2 Ring	ND	ND	0.94	7.94	11.18	22.12	21.10	11.1	13.9
3 Ring	ND	ND	ND	ND	ND	ND	ND	9.0	11.8
4 Ring	ND	ND	ND	ND	ND	ND	ND	0.5	4.5
5 Ring	ND	ND	ND	ND	ND	ND	ND	ND	0.5
6 Ring	ND	ND	ND	ND	ND	ND	ND	ND	ND
Total Cycloparaffins	25.78	41.17	40.42	36.65	41.49	44.48	45.90	35.4	44.4
Aromatics									
Alkyl Benzenes	6.24	10.56	19.05	18.84	14.40	10.29	7.06	9.5	10.4
Naphthalene Benzenes	ND	0.01	0.09	0.28	1.29	8.09	8.80	8.9	5.6
Dinaphthene Benzenes	ND	ND	ND	ND	ND	ND	ND	4.8	3.3
Napthalenes	ND	ND	0.07	0.44	0.15	1.64	7.38	4.4	14.0
Acenaphthenes, Biphenyls	ND	ND	ND	ND	ND	ND	ND	1.9	4.9
Acanaphthalenes, Fluorenes	ND	ND	ND	ND	ND	ND	2.73	0.6	0.2
Phenanthrenes, Anthracenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Naphthene Phenanthrenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Pyrenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Chrysenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Perylenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Dibenzo Anthracenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Benzothiophenes	ND	ND	ND	ND	ND	0.94	1.29	ND	1.0
Dibenzothiophenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Naphthobenzothiophenes	ND	ND	ND	ND	ND	ND	ND	ND	ND
Total Aromatics	6.24	10.57	19.21	19.56	15.84	20.96	27.26	30.1	39.4

*Determined by GC

GENERAL COMMENTS

1. Distillation values for Wilmington, CA; Recluse, WY and Prudhoe Bay, AK crudes were obtained via the Bureau of Mines routine distillation method. Distillation values for API Crude Oils C and D were obtained by using a 60-gallon stainless steel still equipped with an 8 ft x 6-1/4 inch packed column; the operating conditions used followed ASTM D-2892. Distillation values for the shale oil samples were obtained via a Penn State distillation column (References 4, 5 and 58).

2. Limited published data on saturates, olefins, naphthenes and aromatics contents of petroleum crudes are now available. However, additional data are being developed and computerized by DOE, BETC on the weight percents of these constituents in numerous domestic and foreign crudes.

3. Although data are not available for tabular presentation, crude shale oils from surface retorting processes generally contain higher levels of olefins and aromatics than petroleum crudes, and consist of approximately 20% alkanes, 20% aromatics, 25% aromatic resins, and 25% olefins and naphthenes. In-situ oils are generally lower in olefins content and higher in saturated hydrocarbon contents than surface-retorted shale oils (Reference 30).

4. Individual compound identification has been performed on the light (i.e., 55 to 380°F) boiling fraction of Alaskan North Slope crude. Over 70 compounds were identified of the following types: normal and branched alkanes, cycloparaffins, olefins and alkyl benzenes. Individual compound identification by capillary gas chromatographic analysis performed on the light boiling (120-350°F) distillation cuts of two other petroleum crudes under API Project PS-8-GST-(989-300) gave similar results (References 6 and 79).

5. Individual compound identification has been carried out on 3 shale-derived unrefined naphthas (i.e., not less than 10% distilling below 347°F and not less than 95% distilling below 464°F), which can be considered light distillation cuts. Over 70 individual compounds were identified, of the same types as in the comparable petroleum cut described above (i.e., normal and branched alkanes, cycloparaffins, olefins, and alkyl benzenes). A greater number and concentration of olefins (both linear and cyclic) and aliphatic substituted benzenes (e.g., 1-methyl-3-ethyl benzene) were present in the shale-derived samples than in the petroleum samples (Reference 48).

6. Individual sulfur compound analyses carried out on the 0° to approximately 400°C boiling range of various domestic and foreign crude oils (e.g., Wilmington, Wasson, and Agha Jari crudes) resulted in identification of over 200 sulfur-containing compounds of the following types: (a) alkylthiols: C_1H_3SH to $C_8H_{17}SH$; (b) cycloalkylthiols: C_5H_9SH to $C_6H_{11}SH$); (c) alkyl sulfides: C_3H_8SH to $C_8H_{18}S$; (d) cyclic sulfides: C_4H_8S to $C_8H_{16}S$; (e) alkyl-cycloalkyl sulfides: $C_8H_{16}S$ to $C_{10}H_{20}S$; (f) alkyl-arylsulfides: $C_{10}H_{14}S$ (3 isomers); (g) one thienyl sulfide: $C_8H_{12}S_2$; (h) dithiaalkyl sulfides: $C_2H_6S_2$ to $C_4H_{10}S_2$; (i) bicyclic sulfides: $C_7H_{12}S$ to $C_{11}H_{20}S$; (j) one tricyclic sulfide: $C_9H_{14}S$; (k) alkyl thiophenes: C_4H_4S to $C_9H_{14}S$; (l) bicyclic thiophenes: $C_7H_6S_2$ (two isomers); (m) benzothiophenes: C_8H_6S to $C_{10}H_{10}S$; (n) dibenzothiophenes and (o) tricyclic thiophenes. The majority of the sulfur compounds identified have boiling points below 200°F (Reference 7).

7. Approximately 0.94, 1.29 and 1.0 volume percent of various benzothiophenes were identified the 380-400°F, 480-520°F and 600-700°F boiling ranges of an Alaskan North Slope crude oil by mass spectrometry. No dibenzothiophenes or naphthobenzothiophenes were detected in the entire 55°-700°F boiling range of the crude (Reference 6).

8. Analysis of four raw shale oils (Paraho, Geokinetics, Occidental, and Rio Blanco) by liquid chromotography, gas chromatography and mass spectrometry resulted in identification of the following sulfur heterocycles: C_2- through C_5-benzo(6)thiophene, C_1- through C_5-dihydrobenzo(b)-thiophene, dibenzothiophene, C_1- and C_2-dibenzothiophene, phenanthro-(4,5-bcd) thiophene, C_1-phenanthro (4,5-bcd) thiophene, and various 4-ring isomers (Reference 78).

9. Individual oxygen compound analyses carried out on the 0° to approximately 400°C boiling range of 12 domestic and foreign crude oils resulted in identification of over 65 oxygen-containing compounds of the following types: (a) saturated fatty acids: HCOOH to $C_{20}H_{41}COOH$; (b) cycloalkanecarboxylic acids: C_5H_9COOH to $C_9H_{17}COOH$; (c) cycloalkaneacetic acids: $C_6H_{11}COOH$ to $C_9H_{17}COOH$; (d) ketones: C_2H_6CO to R-$C_{13}H_8O$; (e) phenols: C_6H_5OH to $C_{10}H_7OH$; and (f) miscellaneous compounds: $C_6H_6O_3$ to $C_{29}H_{46}O_2$. The majority of the oxygen compounds have boiling points below 200°C (Reference 29).

10. Phenol, alkylphenols (e.g., o-cresol, m-cresol, dimethylphenol and trimethylphenol isomers, o-methylalkylphenol and dimethlyalkylphenol isomers), naphthols (methyl-1-naphthol and dimethyl naphthol) and various methyl ketones (including a C_{16} and C_{23} ketone) were detected in Kerosene Creek, Austraila and Ramsay Crossing, Australia raw shale oils by liquid chromatography followed by gas chromatography and mass spectrometry (Reference 60).

11. Over 40 compound classes of carboxylic acids ranging from C_{16} to C_{31}, and including numerous individual carboxylic acids such as the C_{22} to C_{24} steroid acids of 5 -pregnane-20 -carboxylic acid and 5 - and 5 -cholanic acid, have been identified in petroleum crude using ion exchange separation and GCMS procedures developed at Chevron Research Co., Richmond, CA (Reference 61).

12. The following sulfur compound contents were identified in various boiling cuts of shale oil materials: (a) 4.2 vol. % in crude Paraho - SOHIO Toledo shale oil, and 2.6 vol. % in-situ, Rock Springs, WY crude shale oil in the IBP-400°F cut; (b) 9.2 wt. % crude Paraho - SOHIO Toledo shale oil, and 7.1 wt. % in in-situ, Rock Springs, WY crude shale oil in the 400-650°F cut; and (c) 13.9 wt. % in crude Paraho - SOHIO Toledo shale oil, and 8.1 wt. % in in-situ, Rock Springs WY crude shale oil in the 650-850°F cut (Reference 35).

13. The following oxygen and nitrogen compound values were determined in various boiling cuts of shale oil materials: (a) 2.7 vol. % in crude Paraho - SOHIO Toledo shale oil and 15.1 vol. % in in-situ, Rock Springs, WY crude shale oil in the IBP to 400°F cut; (b) 10.9 wt. % in crude Paraho - SOHIO Toledo shale oil and 9.3 wt. % in in-situ, Rock Springs, WY crude shale oil, and 2.9 wt. % in Paraho - SOHIO Toledo shale oil in the to 400-650°F cut; (c) 33.9 wt. % in crude Paraho - SOHIO Toledo shale oil, 3.1 wt. % in in-situ, Rock Springs, WY crude shale oil, and 6.4 wt. % in Paraho - SOHIO Toledo hydrotreated shale oil in the 650-850°F cut, and (d) 47.9 wt. % in crude Paraho - SOHIO Toledo shale oil, 44.4 wt. % in-situ, Rock Springs, WY crude shale oil, and 6.8 wt. % in Paraho - SOHIO Toledo hydrotreated shale oil in the 850°F+ cut (sulfur-containing compounds included) (Reference 35).

14. The following weight percents of sulfur and oxygen have been reported for various boiling fractions of API crude oils C and D, respectively: (a) 0.014 and 0.0260 (sulfur), and <0.01 and <0.01 (oxygen) in the 120-350°F cut; (b) 0.077 and 4.10 (sulfur), and 0.03 and 0.055 (oxygen) in the 350-550°F cut; (c) 1.8 and 18.7 (sulfur), and 1.8 and <0.01 (oxygen) in the 550-700°F cut; and (d) 2.7 and 29.8 (sulfur), and 4.7 and 2.2 (oxygen) in the 700-1070°F cut (Reference 58).

Part II. Naphtha

Table 54. Specific Gravity

Material	Value	Sample Description/Source	Reference
Petroleum naphtha	0.7603	API data for varnish makers' and painters' naphtha	62
Shale naphtha	NA	--	--

Table 55. API Gravity

Material	Value (degrees)	Sample Description/Source	Reference
Petroleum naphtha	58.8*	Average of 852 unleaded gasolines (antiknock index (R+M/2) below 90)	12
	56.6*	Average of 137 unleaded gasolines (antiknock index (R+M/2) 90.0 and above)	12
	60.3*	Average of 834 regular grade unleaded gasolines	12
	60.4*	Average of 239 premium grade unleaded gasolines	12
	61	Suntech typical gasoline	63
	59.3	Unleaded commercial gasoline average, 1976 DuPont Road octane survey	63
	61.1 (60°F)	Phillips Petroleum Co. unleaded gasoline blend	76
	58.4 (60°F)	Texaco Fire Chief gasoline	77
Shale naphtha	54.7	Paraho-SOHIO Toledo gasoline	33

Explanatory Note

*Determined via ASTM D-287

Table 56. Density

Material	Value (g/ml)*	Sample Description/Source	Reference
Petroleum naphtha	0.7814	E. Wilmington CA crude	57
Shale naphtha	0.7620	Paraho-SOHIO Toledo "weathered gas" feedstock	57
	0.7548	NA	57

Explanatory Note

*Determined by ASTM D-1481-62

Table 57. Reid Vapor Pressure

Material	Value	Sample Description/Source	Reference
Petroleum naphtha	9.8 lb*	Average of 852 unleaded gasolines (antiknock index (R+M/2) below 90)	12
	9.9 lb*	Average of 137 unleaded gasolines (antiknock index (R+M/2) 90.0 and above)	12
	9.9 lb*	Average of 834 regular grade unleaded gasolines	12
	10.1 lb*	Average of 239 premium grade unleaded gasolines	12
	10 lb	Suntech typical gasoline	63
	9.9 lb	Unleaded commercial gasoline average, 1976 DuPont Road octane survey	63
	10.2 psia	Phillips Petroleum Co. unleaded gasoline blend	76
	6.3 psia	Texaco Fire Chief gasoline	77
Shale naphtha	11.9 psi	Paraho-SOHIO, Gary Western	52
	2.1 psi	NA	57

Explanatory Note

*Determined via ASTM D-323

Table 58. Distillation Data

Material	Value (% Evaporation)*	Sample Description/Source	Reference
Petroleum naphtha	89°F - IBP 105°F - 5 120°F - 10 145°F - 20 171°F - 30 221°F - 50 266°F - 70 336°F - 90 370°F - 95 412°F - EP	Average pf 852 unleaded gasolines (antiknock index (R+M/2) below 90)	12
	89°F - IBP 107°F - 5 120°F - 10 146°F - 20 172°F - 30 221°F - 50 261°F - 70 324°F - 90 357°F - 95 400°F - EP	Average of 137 unleaded gasolines (antiknock index (R+M/2) 90.0 or above)	12
	90°F - IBP 105°F - 5 118°F - 10 138°F - 20 159°F - 30 206°F - 50 264°F - 70 343°F - 90 378°F - 95 417°F - EP	Average of 834 regular grade unleaded gasolines	12
	89°F - IBP 104°F - 5 118°F - 10 142°F - 20 166°F - 30 212°F - 50 259°F - 70 334°F - 90 369°F - 95 410°F - EP	Average of 239 premium grade unleaded gasolines	12

(Continued)

Table 58 (Continued)

Material	Value (% Evaporation)*	Sample Description/Source	Reference
Petroleum naphtha	88°F - IBP 115°F - 10 220°F - 50 340°F - 90 425°F - EP	Suntech typical gasoline	63
	92°F - IBP 124°F - 10 220°F - 50 332°F - 90 412°F - EP	Unleaded commercial gasoline average, 1976 DuPont Road Octane Survey	63
	123°F - 10 199°F - 50 325°F - 95 383°F - 100	Phillips Petroleum Co. unleaded gasoline blend	76
	80°F - IBP 160°F - 10 217°F - 50 295°F - 90 340°F - 100	Texaco Fire Chief gasoline	77
	244°F - IBP 247°F - 1 250°F - 3,5 251°F - 10 253°F - 20 254°F - 30 255°F - 40 257°F - 50 259°F - 60 260°F - 70 264°F - 80 269°F - 90 277°F - 95 304°F - EP†	API data for varnish makers' and painters' naphtha	62

(Continued)

Table 58 (Concluded)

Material	Value (% Evaporation)*	Sample Description/Source	Reference
Shale naphtha	86°F - IBP	Paraho-SOHIO Gary Western	52
	136°F - 10		
	192°F - 50		
	342°F - 90		
	395°F - EP		
	200°F - IBP	Paraho-SOHIO Toledo	33
	249°F - 10		
	283°F - 50		
	317°F - 90		
	370°F - EP‡		

Explanatory Notes

*Determined by ASTM D-86

†99% recovered, 1% residue

‡98% recovered, 1% residue, 1% loss

Table 59. GC Simulated Distillation Data*

Material	Boiling Point Range (°C)	Sample Description/Source	Reference
Petroleum naphtha	5% recovered - 58 50% recovered - 139 95% recovered - 206	E. Wilmington, CA crude	57
Shale naphtha	5% recovered - 93 50% recovered - 143 95% recovered - 176	Paraho-SOHIO Toledo "weathered gas" feedstock	57
	5% recovered - 117 50% recovered - 171 95% recovered - 213	NA	57

Explanatory Note

*GC simulated distillation involves use of gas chromatograph rather than distillation column. Retention times of sample peaks are based on retention times of a calibration mixture of C_3 to C_{42} normal paraffins. The boiling range distribution of the sample is calculated in weight percent via computer. Volume percent values are calculated from a density - boiling point correlation of normal paraffins (Reference 35).

Table 60. Refractive Index

Material	Value	Sample Description/Source	Reference
Petroleum naphtha	1.42198 (20°C)	API data for varnish makers' and painters' naphtha	62
Shale naphtha	NA	--	--

Table 61. Molecular Weight

Material	Value (g/mole)	Sample Description/Source	Reference
Petroleum naphtha	114*	API data for varnish makers' and painters' naphtha	62
Shale naphtha	NA	--	--

Explanatory Note

*Mean molecular weight from mass spectrometry data

Table 62. Total Acid Number

Material	Value (mg KOH/g)	Sample Description/Source	Reference
Petroleum naphtha	0.11	E. Wilmington, CA crude	57
Shale naphtha	NA	--	--
	0.02	NA	57

Table 63. Gum Content

Material	Value (mg/100 ml)*	Sample Description/Source	Reference
Petroleum naphtha	1	Average of 852 unleaded gasolines (antiknock index (R+M/2) below 90)	12
	1	Average of 137 unleaded gasolines (antiknock index (R+M/2) 90.0 and above)	12
	1	Average of 834 regular grade unleaded gasolines	12
	2	Average of 239 premium grade unleaded gasolines	12
	1	Suntech typical gasoline	63
	1	Unleaded commercial gasoline average, 1976 DuPont Road octane survey	63
	0.57	Phillips Petroleum Co. unleaded gasoline blend	76
Shale naphtha	NA	--	--

Explanatory Note

*Determined by ASTM D-381.

Table 64. Oxygen Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum naphtha	0.038	E. Wilmington, CA crude	57
Shale naphtha	0.008	Paraho-SOHIO Toledo "weathered gas" feedstock	57
	0.053	NA	57

Table 65. Sulfur Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum naphtha	0.085	E. Wilmington, CA crude	57
	0.028	Average of 852 unleaded gasolines (antiknock index (R+M/2) below 90)	12
	0.019	Average of 137 unleaded gasolines (antiknock index (R+M/2) 90.0 and above)	12
	0.049	Average of 834 regular grade unleaded gasolines	12
	0.034	Average of 239 premium grade unleaded gasolines	12
	<0.005	Suntech typical gasoline	63
	0.0127	Phillips Petroleum Co. unleaded gasoline blend	76
	0.0075	Texaco Fire Chief gasoline	77
Shale naphtha	0.0003	Paraho-SOHIO Toledo "weathered gas" feedstock	57
	0.007	Paraho-SOHIO Gary Western	52
	0.0050	NA	57

Table 66. Nitrogen Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum naphtha	0.001	E. Wilmington, CA crude	57
Shale naphtha	0.089	Paraho-SOHIO Toledo "weathered gas" feedstock	57
	0.03	Paraho-Gary Western	52
	0.00005	NA	57

Table 67. Carbon Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum naphtha	NA	--	--
Shale naphtha	85.7	Paraho-SOHIO Toledo "weathered gas" feedstock	57

Table 68. Hydrogen Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum naphtha	NA	--	--
Shale naphtha	14.3	Paraho-SOHIO Toledo "weathered gas" feedstock	57

Table 69. Trace Elements Content (ppmw)*

Material	Al	Sb	As	Be	Cd	Ca	Cl	Co	Cr	Cu
Petroleum naphtha†	<0.001 to 0.02	<0.003 to 0.05	<0.001 to 0.002	<0.001	<0.001 to 0.03	<0.06 to 0.26	<0.02 to 0.80	NA	<0.001 to 0.34	<0.011 to 0.25
	<0.007	<0.007 to 0.5	<0.004 to 0.009	<0.001	<0.08	<0.06 to 3.0	<0.05 to 1.10	NA	<0.003 to 0.03	0.010 to 0.40
	NA	<0.10	<0.1	<0.001	<0.01	<0.2 to 0.7	<0.007 to 0.90	NA	<0.005 to 0.016	0.06 to 0.20
	NA	<0.5	<0.3	NA	0.03	NA	NA	NA	<0.05	<0.05
Shale naphtha	0.031 (NAA)	ND(<3) (XRF)	ND(<0.5) (XRF)	<0.01 (AA)	<0.03 (AA)	ND(<0.6) (NAA)	ND(<2) (XRF)	<0.07 (FE)	ND(≤0.1) (NAA)	0.03 (AA)
	NA	<0.5	0.9	NA	<0.03	NA	NA	NA	<0.05	<0.05

(Continued)

Table 69 (Continued)

Material	Fe	Pb‡	Mg	Mn	Hg	Mo	Ni	Se	Si	Ag	Na
Petroleum naphtha	0.07 to 6.00	238 to 763	<0.002 to 0.004	0.002 to 0.03	NA	NA	0.003 to 1.5	<0.06	NA	<0.002 to 0.03	NA
	0.07 to 3.80	190 to 750	<0.002 to 0.01	0.001 to 0.011	NA	NA	0.001 to 0.07	<0.06	NA	<0.54	NA
	0.3 to 13.0	132 to 135	NA	<0.002 to 0.03	NA	NA	0.03 to 2.00	<0.04	NA	<0.1	NA
	<0.05	<0.06	NA	NA	<1	NA	<0.05	<0.3	NA	NA	NA
Shale naphtha	<0.01 (FE)	<0.07 (AA)	ND(≤5.3) (NAA)	<0.03 (AA)	ND(<2) (XRF)	ND(≤0.032) (NAA)	ND(≤1.7) (NAA)	ND(<0.5) (XRF)	ND(≤7.0)	<0.03 (AA)	0.08 (FE)
	<0.05	<0.06	NA	NA	<1	NA	<0.05	<0.3	NA	NA	NA

(Continued)

Table 69 (Concluded)

Material	Sr	Th	Sn	Ti	V	Zn	Sample Description/Source	Reference
Petroleum naphtha	NA	NA	<0.02 to 0.40	NA	0.001 to 0.002	0.001 to 2.00	Range of 22 premium gasolines	13
	NA	NA	<0.01 to 0.2	NA	<0.007	0.010 to 2.00	Range of 22 regular gasolines	13
	NA	NA	<0.6	NA	<0.003	0.20 to 0.50	Range of 6 low lead gasolines	13
	NA	NA	NA	NA	<0.05	<0.05	NA	57
Shale naphtha	ND(<0.8) (NAA)	ND(<6) (XRF)	ND(<1.5) (NAA)	ND(<0.4) (XRF)	ND(<0.0008) (NAA)	<0.03 (AA)	Paraho - SOHIO Toledo "weathered gas" feedstock	35
	NA	NA	NA	NA	<0.05	0.07	NA	57

Explanatory Notes

*Methods used include atomic absorption spectroscopy (AA), flame emission spectroscopy (FE), neutron activation analysis (NAA), and X-ray fluorescence (XRF).

†The following data on phosphorous content are available for petroleum naphtha: (a) 0.005 g/gal detected in Suntech typical gasoline; (b) 1 ppm detected in Phillips Petroleum Co. unleaded gasoline blend, (References 63 and 76, respectively).

‡The following additional data on lead content of petroleum naphtha are available: (a) <0.0005 g/gal Pb detected in Suntech typical gasoline; (b) 0.00004 g/gal Pb detected in Phillips Petroleum Co.unleaded gasoline blend; and (c) 1.94 g/gal detected in Texaco Fire Chief gasoline, (References 63, 76 and 77, respectively).

Table 70. Saturates, Olefins and Aromatics Contents

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum naphtha			
A. Saturates	66[*]	Suntech typical gasoline	63
	66[*]	Unleaded commercial gasoline average, 1976 DuPont Road Octane Survey	63
	67.7	Phillips Petroleum Co. unleaded gasoline blend	76
	64.8	Texaco Fire Chief gasoline	77
	55.4	API data for varnish makers' and painters' naphtha	62
	62 (wt %)	Average of 15 premium gasolines, Pedco Survey, 1969	13
B. Olefins	8[*]	Suntech typical gasoline	63
	7[*]	Unleaded commercial gasoline average, 1976 DuPont Road Octane Survey	63
	8.3	Phillips Petroleum Co. unleaded gasoline blend	76
	7.8	Texaco Fire Chief gasoline	77
	11 (wt %)	Average of 15 premium gasolines, Pedco Survey, 1969	13
	32.7[†]	API data for varnish makers' and painters' naphtha	62
C. Aromatics	26[*,‡]	Suntech typical gasoline	63
	27[*]	Unleaded commercial gasoline average, 1976 DuPont Road Octane Survey	63
	24.0	Phillips Petroleum Co. unleaded gasoline blend	76
	27.4	Texaco Fire Chief gasoline	77
	27 (wt %)	Average of 15 premium gasolines, Pedco Survey, 1969	13
	11.7[§]	API data for varnish makers' and painters' naphtha	62

(Continued)

Table 70 (Concluded)

Material	Value (Vol. %)	Sample Description/Source	Reference
Shale naphtha			
A. Saturates	52.0	Paraho-SOHIO Gary Western	52
	83.7	Paraho-SOHIO Toledo "weathered gas" feedstock	35
B. Olefins	36	Paraho-SOHIO Gary Western	52
	2.6	Paraho-SOHIO Toledo "weathered gas" feedstock	35
C. Aromatics	13.7	Paraho-SOHIO Toledo "weathered gas" feedstock	35
	0.061 wt % benzene	--	57

Explanatory Notes

*Determined by ASTM D-1319

†Includes 30.3 vol % monocycloparaffins and 2.4 vol % dicycloparaffins.

‡Benzene content is 0.8 vol. %

§Benzene and indans + tetralins contents are each 0.1 vol %.

Table 71. Detailed Hydrocarbon Class Analysis

Material	Compound Class	Value Vol. %	Sample Description/Source	Reference
Petroleum naphtha	NA	--	--	-
Shale naphtha	Paraffins	44.0	Paraho-SOHIO Gary Western	52
	Naphthenes	8.0		
	Total saturates	52.0		
	N-paraffins	31.1	Paraho-SOHIO Toledo "weathered gas" feedstock	35
	Iso-paraffins	19.2		
	Total paraffins	50.3		
	Cyclopentanes	13.2		
	Cyclohexanes	19.0		
	Total monocycloparaffins	32.2		
	Total dicycloparaffins	1.2		
	Total saturates	83.7		
	Benzene	0.2		
	Toluene	1.7		
	C_8 aromatics	4.7		
	C_9 aromatics	5.8		
	C_{10} aromatics	0.8		
	Total alkylbenzenes	13.2		
	Total indans & tetralins	0.5		
	Total aromatics	13.7		
	Paraffins	49.95	Paraho-SOHIO Toledo gasoline	33
	Monocycloparaffins	31.62		
	Dicycloparaffins	2.40		
	Alkylbenzenes	15.20		
	Indans & tetralins	0.51		
	Naphthalenes	0.32		

Table 72. Nitrogen Compound Class Analysis - Solvent Fractionation ("Type 1")*

Material	Compound Class	Number of Carbons in Side Chain	Number of Isomers Detected	Relative Amount of Class	Sample Description/Source	Reference
Petroleum naphtha		NA	NA	NA	--	--
Shale naphtha[†]						
	Piperdines ($C_nH_{2n+1}N$)	2	2		Paraho-SOHIO Toledo	64
		3	3	7%		
	Pyridines ($C_nH_{2n-5}N$)	1	1	ND		
		2	4	ND		
		3	10	ND		
		4	8	93%		
		5	3	ND		

Explanatory Notes

* This solvent fractionation method involves acid extraction followed by GC-MS analysis; details of the method can be found in Reference 64.

[†] Over 30 nitrogen containing compounds were detected; the average molecular weight of the compounds was 125.

GENERAL COMMENTS

1. Commercial naphtha is a refined, partly refined or unrefined petroleum or shale oil product comprised mostly of gasoline, not less than 10 percent of which distills below 347°F and not less than 95 percent of which distills below 464°F. Hydrocarbon compound classes and individual hydrocarbon compounds found in light boiling (i.e., less than 464°F) petroleum or shale oil distillation fractions (see data presented in Tables 22, 23 and 24) can be expected to be present in product naphtha in varying degrees, depending on the nature and extent of the refining used.

2. Results of individual compound identifications performed on 15 premium, 36 regular and other petroleum gasolines indicate the presence of the following compounds: (a) paraffins - C_1 to C_8 normal alkanes and mono-, di- and/or trimethyl substituted analogs; (b) naphthenes - including methylcyclopentane, cyclohexane, and methylcyclohexane; (c) olefins - including methyl butene, pentene and methyl pentene; and (d) aromatics - benzene, toluene, ethylbenzene, xylenes, propylbenzene, methylethylbenzenes and trimethylbenzene (Reference 13).

3. In a separate study, a typical petroleum premium gasoline was found to contain 180 individual hydrocarbon compounds of the classes listed in Note 2 (Reference 13).

4. Although no data are available on the PNA content of naphtha products, it is reasonable to assume that very low levels of certain PNA's may be present since various triaromatics, tetraaromatics and higher boiling compounds have been found in the lower boiling (<500°F) fractions of petroleum crudes and hydrotreated shale oils (see Table 36).

5. Data are unavailable on the nitrogen, sulfur and oxygen compounds in naphtha products. However, it is likely that very low levels of various pyridines, pyrroles and other nitrogen-containing compounds, as well as various thiols, sulfides, carboxylic acids, ketones and other sulfur- and oxygen-containing compounds may be present, based on data presented for low boiling (<400°F) fractions of petroleum crudes and hydrotreated shale oils (see Part I).

Part III. Jet Fuel

Table 73. Specific Gravity

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel			
JP-5	0.8170	Average of several aviation turbine fuels	16
	0.8142	NAPTC	18
Shale jet fuel			
JP-4	0.7507	Paraho-SOHIO Gary Western	38
JP-5	0.8081 (60°F)	Paraho-SOHIO Toledo	67
JP-8	0.8044 (60°F)	Paraho-SOHIO Toledo	67
Jet A	0.8054, 0.7927, 0.8026 (60°F)	Paraho-SOHIO Toledo	51

Table 74. API Gravity

Material	Value (degrees)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	53.5*	Average of 26 samples	21
JP-5	41.2*	Average of 7 samples	21
Jet A	42.7	Average of several aviation turbine fuels	21
	42.3	NA	18
Jet A	42.7	Average of 60 samples	21
Shale jet fuel			
JP-4	57.0	Paraho-SOHIO Gary Western	38
	50.2, 49.6	Geokinetics-HRI	34
JP-5	44	Paraho-SOHIO Gary Western	38
	43.6	Paraho-SOHIO Toledo	33
JP-8	44.4	Paraho-SOHIO Toledo	67
Jet A	44.2, 47.0, 44.8	Paraho-SOHIO Toledo	51

Explanatory Notes

*Determined via ASTM D-287

Table 74. API Gravity

Material	Value (degrees)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	53.5*	Average of 26 samples	21
JP-5	41.2*	Average of 7 samples	21
Jet A	42.7	Average of several aviation turbine fuels	21
	42.3	NA	18
Jet A	42.7	Average of 60 samples	21
Shale jet fuel			
JP-4	57.0	Paraho-SOHIO Gary Western	38
	50.2, 49.6	Geokinetics-HRI	34
JP-5	44	Paraho-SOHIO Gary Western	38
	43.6	Paraho-SOHIO Toledo	33
JP-8	44.4	Paraho-SOHIO Toledo	67
Jet A	44.2, 47.0, 44.8	Paraho-SOHIO Toledo	51

Explanatory Notes

*Determined via ASTM D-287

Table 75. Viscosity

Material	Value (Centistokes)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-5	10.4*	Average of 5 samples	21
	10.5	Average of several aviation turbine fuels	21
	9.34 (-22°F)	NA	18
Jet A	8.8*	Average of 48 samples	21
Shale jet fuel			
JP-5	1.352 (104°F)†	Paraho-SOHIO Toledo	35
	4.68 (-4F)	Paraho-SOHIO Toledo	67
	14.8 (-30°F)	Sohio-Gary Western	38
JP-8	1.299 (104°F)†	Paraho-SOHIO Toledo	35
	4.19 (-4°F)	Paraho-SOHIO Toledo	67
Jet A	10.38, 9.39, 10.09	Paraho-SOHIO Toledo	51

Explanatory Notes

*Determined via ASTM D-445 at -30°F
†Determined via ASTM D-445

Table 76. Pour Point

Material	Value (°F)*	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	-60	Paraho-SOHIO Toledo	35
JP-8	-60	Paraho-SOHIO Toledo	35

Explanatory Note

*Determined via ASTM D-97.

Table 77. Density

Material	Value (g/ml)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	0.8175	NA	57
Jet A	0.8443*	E. Wilmington, CA crude	57
Shale jet fuel			
JP-5	0.8068*	Paraho-SOHIO Toledo	35
JP-8	0.8036	Paraho-SOHIO Toledo	35
	0.7937*	NA	57

Explanatory Note

*Determined via ASTM D-1481

Table 78. Reid Vapor Pressure

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	2.5 lb*	Average of 23 samples	21
Shale jet fuel			
JP-4	2.0 psi	Paraho-SOHIO Gary Western	38
	2.30, 2.50 psi	Geokinetics-HRI	34
	<0.1 psi	NA	57

Explanatory Notes

*Determined via ASTM D-323

Table 79. Distillation Data

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	139°F - IBP*	Average of 26 samples	21
	208°F - 10		
	234°F - 20		
	293°F - 50		
	388°F - 90		
	451°F - EP		
JP-5	346°F - IBP*	Average of 7 samples	21
	387°F - 10		
	398°F - 20		
	423°F - 50		
	470°F - 90		
	509°F - EP		
	362°F - IBP	NA	52
	390°F - 10		
	422°F - 50		
	480°F - 90		
	502°F - EP		
	356°F - IBP	NA	18
	374°F - 5		
	380°F - 10		
	386°F - 20		
	394°F - 30		
	400°F - 40		
	410°F - 50		
	418°F - 60		
	430°F - 70		
	442°F - 80		
	460°F - 90		
	480°F - 95		
	508°F - EP		
Jet A	345°F - IBP	Average of 60 samples	21
	375°F - 10		
	387°F - 20		
	416°F - 50		
	473°F - 90		
	518°F - EP		

(Continued)

Table 79 (Continued)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum jet fuel			
	325°F - IBP	API	65
	361°F - 5		
	376°F - 10		
	392°F - 20		
	405°F - 30		
	416°F - 40		
	427°F - 50		
	439°F - 60		
	453°F - 70		
	469°F - 80		
	488°F - 90		
	506°F - 95		
	540°F - EP[#]		
Shale jet fuel			
JP-4	161, 185°F - IBP[*]	Geokinetics-HRI	34
	225, 221°F - 5		
	264, 255°F - 10		
	294, 294°F - 20		
	333, 323°F - 30		
	354, 249°F - 40		
	374, 370°F - 50		
	390, 386°F - 60		
	405, 405°F - 70		
	422, 426°F - 80		
	448, 452°F - 90		
	480, 478°F - 95		
	509, 508°F - EP[‡]		
JP-5	342°F - IBP	Paraho-Gary Western	52
	376°F - 10		
	426°F - 50		
	492°F - 90		
	514°F - EP		
	354°F - IBP	Paraho-SOHIO Toledo	67
	372°F - 10		
	378°F - 20		
	396°F - 50		
	442°F - 90		
	478°F - EP[††]		
	370°F - IBP	Paraho-SOHIO Toledo	33
	384°F - 10		
	400°F - 50		
	436°F - 90		
	480°F - EP		

(Continued)

Table 79 (Concluded)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Shale jet fuel			
JP-8	352°F - IBP 369°F - 10 372°F - 20 394°F - 50 441°F - 90 495°F - EP#	Paraho-SOHIO Toledo	67
Jet A	342, 333, 332°F = IBP 382, 386, 378°F - 10 394, 378, 385°F - 20 419, 407, 415°F - 50 462, 447, 455°F - 90 504, 515, 507°F - EP**	Paraho-SOHIO Toledo	51
Union jet fuel	NA	--	--

Explanatory Notes

*Determined via ASTM D-86

†98% recovery, 1% residue

‡1% residue, 1% loss

§98.5% recovery, 1.5% residue

#98.5% recovery, 1.0% residue, 0.5% loss

**1.5, 1.0, 1.0% residue; 0, 0, 0.5% loss, respectively

Table 80. GC Simulated Distillation Data*

Material	Boiling Point Range (°C)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-5	5% recovered - 197 50% recovered - 217 95% recovered - 243	Average of several aviation turbine fuels	16
Jet A	5% recovered - 160 50% recovered - 230 95% recovered - 275	E. Wilmington, CA crude	57
Shale jet fuel			
JP-5	5% recovered - 171 50% recovered - 208 95% recovered - 253	Paraho-SOHIO Toledo	57
	0.1% recovered - 136.5 1% recovered - 159.7 10% recovered - 174.5 20% recovered - 185.3 50% recovered - 208.9 90% recovered - 245.9 95% recovered - 255.0 99% recovered - 278.8 99.5% recovered - 291.6	Paraho-SOHIO Toledo	67
JP-8	0.1% recovered - 120.1 1% recovered - 153.6 10% recovered - 170.4 20% recovered - 176.6 50% recovered - 203.1 90% recovered - 241.0 95% recovered - 252.2 99% recovered - 274.6 99.5% recovered - 285.7	Paraho-SOHIO Toledo	67
	5% recovered - 150 50% recovered - 219 95% recovered - 270	NA	57

Explanatory Note

*GC simulated distillation involves use of gas chromatograph rather than distillation column. Retention times of sample peaks are based on retention times of a calibration mixture of C_3 to C_{42} normal paraffins. The boiling range distribution of the sample is calculated in weight percent via computer. Volume percent values are calculated from a density - boiling point correlation of normal paraffins (Reference 35).

Table 81. Refractive Index

Material	Value (Abbe Refractometer, 67°C)	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	1.4299	Paraho-SOHIO Toledo	35
JP-8	1.4283	Paraho-SOHIO Toledo	35

Table 82. Molecular Weight (Cryoscopic)

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	167	Paraho-SOHIO Toledo	35
JP-8	156	Paraho-SOHIO Toledo	35

Table 82. Molecular Weight (Cryoscopic)

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	167	Paraho-SOHIO Toledo	35
JP-8	156	Paraho-SOHIO Toledo	35

Table 83. Bottom Sediment and Water

Material	Value (Vol. %)*	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	0.05	Paraho-SOHIO Toledo	35
JP-8	<0.05	Paraho-SOHIO Toledo	35

Explanatory Note

*Determined by ASTM D-96

Table 84. Total Acid Number

Material	Value (mg KOH/g)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	0.006*	Average of 23 samples	21
JP-5	0.007*	Average of 6 samples	21
Jet A	0.34	E. Wilmington, CA crude	57
	0.014	Average of 5 samples	21
Shale jet fuel			
JP-4	0.010	Paraho-SOHIO Toledo	38
JP-5	0.047	Paraho-SOHIO Gary Western	38
	0.005	Paraho-SOHIO Toledo	33
	0.0	Paraho-SOHIO Toledo	67
JP-8	0.01	Paraho-SOHIO Toledo	67
Jet A	0.05, 0.03, 0.06	Paraho-SOHIO Toledo	51
	0.00	NA	57

Explanatory Notes

*Determined via ASTM D-974

Table 85. Flash Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-5	154	NA	18
Shale jet fuel			
JP-5	140	Paraho-SOHIO Gary Western	38
	145	Paraho-SOHIO Toledo	67
JP-8	135	Paraho-SOHIO Toledo	67
Jet A	134, 126, 138	Paraho-SOHIO Toledo	51

Table 86. Freezing Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	-79*	Average of 25 samples	21
JP-5	-57*	Average of 7 samples	21
	-69*	Average of several aviation turbine fuels	16
	-58	NA	18
Jet A	-49*	Average of 60 samples	57
	<-76	E. Wilmington, CA crude	57
Shale jet fuel			
JP-4	-91.3	Paraho-SOHIO Gary Western	38
JP-5	-26.0	Paraho-SOHIO Gary Western	38
	-60	Paraho SOHIO Toledo	67
JP-8	-62	Paraho-SOHIO Toledo	67
	-49	NA	57

Explanatory Notes

*Determined via ASTM D-2386

Table 87. Aniline Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	128.7*	Average of 24 samples	21
JP-5	142.5*	Average of 7 samples	21
	144.5	Average of several aviation turbine fuels	16
	61.5	NA	18
Jet A	142.4*	Average of 50 samples	21
Shale jet fuel			
JP-5	140	Paraho-SOHIO Toledo	67
JP-8	144	Paraho-SOHIO Toledo	67
Jet A	151, 161.4, 150.4	Paraho SOHIO Toledo	51

Explanatory Notes

*Determined by ASTM D-611

Table 88. Aniline Gravity Constant

Material	Value (No.)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	6,891	Average of 24 samples	21
JP-5	5,869	Average of 7 samples	21
	6,059	Average of several aviation turbine fuels	16
	6,036	NA	18
Jet A	6,072*	Average of 50 samples	21
Shale jet fuel			
JP-5	6,134	Paraho-SOHIO Toledo	67
JP-8	6,407	Paraho-SOHIO Toledo	67
Jet A	6,674, 7,586 6,738	Paraho-SOHIO Toledo	51

Explanatory Notes

*Average of 26 samples

Table 89. Water Tolerance

Material	Value (ml)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	0.7	Average of 26 samples	21
JP-5	0.7	Average of 3 samples	21
Jet A	0.6	Average of 54 samples	21
Shale jet fuel*	NA	NA	--

Explanatory Notes

*The following "water reaction" data are available for a Paraho-SOHIO Gary Western sample: volume change, 0.0; rating, 1 (Reference 38).

Table 90. Water Separation Index

Material	Value (No.)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	91*	Average of 25 samples	21
JP-5	94*	Average of 6 samples	21
	94	Average of several aviation turbine fuels	16
Jet A	95	Average of 56 samples	21
Shale jet fuel	NA	--	--

Explanatory Notes

*Determined via ASTM D-2550

Table 91. Smoke Point

Material	Value (mm)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	26.0*	Average of 24 samples	21
JP-5	21.9*	Average of 7 samples	21
	23.0	Average of several aviation turbine fuels	16
	23.0	NA	66
	21	NA	18
Jet A	22.6	Average of 57 samples	21
Shale jet fuel			
JP-5	22.0	Paraho-SOHIO Gary Western	66
	17.5	Paraho-SOHIO Toledo	67
JP-8	20.2	Paraho-SOHIO Toledo	67

Explanatory Notes

*Determined by ASTM D-1322

Table 92. Gum Content

	Value (mg/100 ml)			
Material	Existent Gum at 450°F,	Potential Gum at 212°F,	Sample/Description/Source	Reference
Petroleum jet fuel				
JP-4	0.7*	1.0†	Average of 26 and 3 samples, respectively	21
JP-5	0.7*	NA	Average of 7 samples	21
	<7	NA	NA	66
	1.3	NA	Average of several aviation turbine fuels	16
Jet A	1.0*	2.5†	Average of 54 and 18 samples, respectively	21
Shale jet fuel				
JP-4	10	3.6	Paraho-SOHIO Gary Western	38
JP-5	116.2	137.8	Paraho-SOHIO Gary Western	38
	81.7	NA	Paraho-SOHIO Gary Western	66
	1.4	NA	Paraho-SOHIO Toledo	33
	0	NA	Paraho-SOHIO Toledo	67
JP-8	0.4	NA	Paraho-SOHIO Toledo	67
Jet A	5.8, 2.7, 3.1	NA	Paraho-SOHIO Toledo	51

Explanatory Notes

*Determined by ASTM D-381 and D-873
†Determined by ASTM D-873

Table 93. Heat of Combustion

Material	Value (Net, Btu/lb)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	18,702*	Average of 24 samples	21
JP-5	18,530*	Average of 7 samples	21
	18,563	NA	66
	18,526	Average of several aviation turbine fuels	16
	18,551	NA	18
Jet A	18,598*	Average of 53 samples	21
Shale jet fuel			
JP-4	18,337#	Paraho-SOHIO Gary Western	38
JP-5	18,160**	Paraho-SOHIO Gary Western	38
	18,576	Paraho-SOHIO Gary Western	66
	18,395	Paraho-SOHIO Toledo	67
JP-8	18,455	Paraho-SOHIO Toledo	67
Jet A	18,273; 18,322; 18,500	Paraho-SOHIO Toledo	51

Explanatory Notes

*Determined by ASTM D-1405

†Gross heat of combustion, 19,496 Btu/lb

‡Gross heat of combustion, 19,249 Btu/lb

Table 94. Thermal Stability

Material	Value (Pressure Drop, Inches Hg)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	0.4*	Average of 23 samples	21
JP-5	0.2*	Average of 5 samples	21
	"Pass"	NA	18
Jet A	0.3*	Average of 51 samples	21
Shale jet fuel			
JP-4	4 plus	Paraho-SOHIO Gary Western	38
	0	Geokinetics -HRI	34
JP-5	3.0 (260°F)	Paraho-SOHIO Gary Western	38
	0	Paraho-SOHIO Toledo	67
JP-8	0	Paraho-SOHIO Toledo	67

Explanatory Notes

*Determined via ASTM D-1660

Table 95. Corrosion Rating

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel			
JP-5	NA	NA	18
Shale jet fuel			
JP-4	1B at 3 hr/212°F	Paraho-SOHIO Gary Western	38
	1B, 1A	Geokinetics-HRI	34
JP-5	1B at 3 hr/212°F	Paraho-SOHIO Gary Western	38
	1B max at 212°F*	Paraho-SOHIO Toledo	67
JP-8	1A at 212°F*	Paraho-SOHIO Toledo	67
Jet A	2, 1A, 1A*	Paraho-SOHIO Toledo	51

Explanatory Notes

*Copper strip method

Table 96. Water Separation Index, Modified

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-4	46	Paraho-SOHIO Gary Western	38
JP-5	69	Paraho-SOHIO Gary Western	38
	95	Paraho-SOHIO Toledo	33

Table 97. Anti-Icing*

Material	Value	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel†			
JP-4	0.003%	Paraho-SOHIO Gary Western	38
JP-5	0.004%	Paraho-SOHIO Gary Western	38

Explanatory Notes

*Anti-icing levels reflect the amount of additives used and not a significant fuel property.

†JP-4 and JP-5 are military fuels; the military specification MIL-T-5624L requires 0.10 vol % minimum and 0.15 vol % maximum concentration for anti-icer additive for both fuels.

Table 98. Oxygen Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum jet fuel			
Jet A	0.083	E. Wilmington, CA crude	57
Shale jet fuel			
JP-4	0.038	NA	57
JP-5	1.1	Paraho-SOHIO Toledo	35
	0.38	Paraho-SOHIO Toledo	67
JP-8	0.009	Paraho-SOHIO Toledo	35
	0.40	Paraho-SOHIO Toledo	67
Jet A	0.05, 0.05, 0.05	Paraho-SOHIO Toledo	51
	0.025	NA	57

Table 99. Sulfur Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	0.030*	Average of 26 samples	21
JP-5	0.044*	Average of 7 samples	21
	0.11, <0.40	NA	66
	0.096	Average of several aviation turbine fuels	16
	0.05	NA	18
Jet A	0.050*	Average of 60 samples	21
	0.351	E. Wilmington, CA crude	57
Shale jet fuel			
JP-4	0.0013	Paraho-SOHIO Gary Western	38
	<0.01	Geokinetics-HRI	34
	0.0029	NA	57
JP-5	0.0015	Paraho-SOHIO Toledo	57, 35
	0.005	Paraho-SOHIO Toledo	67
	0.0027	Paraho-SOHIO Gary Western	38
	0.05	Paraho-SOHIO Gary Western	66
	0.0001†	In-situ; Rock Springs, WY-LETC	66
	0.0005‡	In-situ; Rock Springs, WY-LETC	66
JP-8	0.00006	Paraho-SOHIO Toledo	35
	0.002	Paraho-SOHIO Toledo	67
Jet A	0.007, 0.005, 0.006	Paraho-SOHIO Toledo	51
	0.0009	NA	57

Explanatory Notes

*Determined via ASTM D-1266
†Multi-step process
††Single step process

Table 100. Nitrogen Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum jet fuel			
Jet A	0.0062	E. Wilmington, CA crude	57
Shale jet fuel			
JP-4	0.014	Paraho-SOHIO Gary Western	38
	0.0013	NA	57
JP-5	0.00005	Paraho-SOHIO Toledo	35
	<0.0001	Paraho-SOHIO Toledo	67
	0.096	Paraho-SOHIO Gary Western	38
	0.086	Paraho-SOHIO Gary Western	66
	0.0079*	In-situ; Rock Springs, WY-LETC	66
	0.0005†	In-situ; Rock Springs, WY-LETC	66
JP-8	0.0022	Paraho-SOHIO Toledo	35
	0.000031	Paraho-SOHIO Toledo	67
Jet A	0.0347, 0.00032, 0.0146	Paraho-SOHIO Toledo	51
	0.0017	NA	57

Explanatory Notes

*Multi-step process

†Single-step process

Table 101. Carbon Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	86.2	Paraho-SOHIO Toledo	35
	85.92	Paraho-SOHIO Toledo	67
JP-8	86.2	Paraho-SOHIO Toledo	35
	86.05	Paraho-SOHIO Toledo	67
Jet A	85.81, 85.43, 85.72	Paraho-SOHIO Toledo	51

Table 102. Hydrogen Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum jet fuel	NA	--	--
Shale jet fuel			
JP-5	13.8	Paraho-SOHIO Toledo	35
	13.74	Paraho-SOHIO Gary Western	66
	13.68	Paraho-SOHIO Toledo	67
JP-8	13.8	Paraho-SOHIO Toledo	35
	13.70	Paraho-SOHIO Toledo	67
Jet A	13.87, 14.42, 13.93	Paraho-SOHIO Toledo	51

Table 103. Trace Elements Content (ppmw)*

Material	Al	Sb	As	Be	Cd	Ca	Cl	Co	Cr	Cu
Petroleum jet fuel										
JP-4	NA	<0.5	0.5	NA	<0.03	NA	NA	NA	<0.05	<0.05
Jet A	NA	1.1	<0.3	NA	<0.03	NA	NA	NA	<0.05	<0.05
Shale jet fuel										
JP-4	NA	<0.5	0.9	NA	<0.03	NA	NA	NA	<0.05	<0.05
JP-5	0.048 (NAA)	ND(<3) (XRF)	<0.5 (XRF)	<0.01 (AA)	<0.02 (AA)	ND(≤0.6) (NAA)	ND(<2) (XRF)	<0.04 (FE)	ND(≤0.094) (NAA)	0.02 (AA)
JP-8	0.056 (NAA)	ND(<3) (XRF)	ND(<0.5) (XRF)	<0.01 (AA)	<0.02 (AA)	ND(≤0.6) (NAA)	ND(<2) (XRF)	<0.06 (FE)	ND(<0.068) (NAA)	<0.02 (AA)
Jet A	NA	<0.5	0.6	NA	<0.03	NA	NA	NA	<0.05	<0.05

(Continued)

Table 103 (Continued)

Material	Fe	Pb	Mg	Mn	Hg	Mo	Ni	Se	Si	Ag	Na
Petroleum jet fuel											
JP-4	<0.05	0.09	NA	NA	<1	NA	<0.05	<0.3	NA	NA	NA
Jet A	<0.05	0.07	NA	NA	<1	NA	<0.05	<0.3	NA	NA	NA
Shale jet fuel											
JP-4	<0.05	<0.06	NA	NA	3†	NA	<0.05	<0.3	NA	NA	NA
JP-5	<0.01 (FE)	<0.06 (AA)	ND(≤5.3) (NAA)	<0.02 (AA)	ND(<2) (XRF)	ND(≤0.03) (NAA)	ND(≤3.9) (NAA)	ND(<0.5) (XRF)	ND(≤10) (NAA)	<0.02 (AA)	0.14 (FE)
Jet A	<0.01 (FE)	<0.06 (AA)	ND(<5.3) (NAA)	<0.02 (AA)	ND(<2) (XRF)	ND(≤0.024) (NAA)	ND(≤1.6) (NAA)	ND(<0.5) (XRF)	ND(≤13) (NAA)	<0.02 (AA)	0.06 (FE)
	<0.05	<0.06	NA	NA	2†	NA	0.08	<0.3	NA	NA	NA

(Continued)

Table 103 (Concluded)

Material	Sr	Th	Sn	Ti	V	Zn	Sample Description/Source	Reference
Petroleum jet fuel								
JP-4	NA	NA	NA	NA	<0.05	<0.05	NA	57
Jet A	NA	NA	NA	NA	<0.05	<0.05	NA	57
Shale jet fuel								
JP-4	NA	NA	NA	NA	<0.05	<0.05	NA	57
JP-5	ND(≤0.94) (NAA)	ND(<6) (XRF)	ND(≤0.93) (NAA)	ND(<0.4) (XRF)	ND(≤0.0008) (NAA)	<0.02 (AA)	Paraho - SOHIO Toledo	35
Jet A	ND≤0.58) (NAA)	ND(<6) (XRF)	ND(<0.87) (NAA)	ND(<0.4) (XRF)	ND(≤0.0008) (NAA)	<0.02 (AA)	Paraho - SOHIO Toledo	35
	NA	NA	NA	NA	<0.05	<0.05	NA	57

Explanatory Notes

*Methods used include atomic absorption spectroscopy (AA), flame emission spectroscopy (FE), neutron activation analysis (NAA), and X-ray fluorescence (XRF).

†Result may be an artifact of laboratory processing, since no mercury was detected in the raw shale oil.

Table 104. Saturates, Olefins and Aromatics Contents

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4 fuel			
Saturates	NA	NA	21
Olefins	1.0*	Average of 26 samples	
Aromatics	13.0*,†	Average of 26 samples	
JP-5			
Saturates	NA	NA	21
Olefins	0.8*	Average of 7 samples	
Aromatics	16.4*	Average of 7 samples	
Saturates	NA	Average of several aviation turbine fuels	16
Olefins	0.8		
Aromatics	16.0		
Saturates	75.98	NA	18
Olefins	3.65	NA	
Aromatics	20.37	NA	
Jet A			
Saturates	NA	NA	21
Olefins	0.9*	Average of 41 samples	
Aromatics	17.9*,‡	Average of 60 samples	
Saturates	82.1	API	65
Olefins	NA		
Aromatics	17.9		
Shale jet fuel			
JP-4			
Saturates	87.9	Paraho-SOHIO Gary Western	38
Olefins	0.4		
Aromatics	11.7		
Saturates	NA	Geokinetics-HRI	34
Olefins	0.5, 0.4		
Aromatics	8.9, 13.5		

(Continued)

Table 104 (Continued)

Material	Value (Vol. %)[*]	Sample Description/Source	Reference
Shale jet fuel			
JP-5			
Saturates	74.7, NA	Paraho-SOHIO Gary Western	38, 66
Olefins	4.3, NA		
Aromatics	21.0, 26.0		
Saturates	43.7, NA	Paraho-SOHIO Toledo[§]	33, 67
Olefins	34.5, 2		
Aromatics	21.8, 22		
Saturates	NA	In-situ; Rock Springs, WY - LETC (multi-step process)	66
Olefins	NA		
Aromatics	23.7		
Saturates	NA	In-situ; Rock Springs, WY - LETC (single-step process)	66
Olefins	NA		
Aromatics	21.3		
JP-8			
Saturates	NA	Paraho-SOHIO Toledo[#]	67
Olefins	2		
Aromatics	21		
Jet A			
Saturates	NA	Paraho-SOHIO Toledo	51
Olefins	0.8, 1.2, 0.7		
Aromatics	17.9, 7.6, 17.2		

(Continued)

Table 104 (Concluded)

Material	Value (Vol. %)[*]	Sample Description/Source	Reference
Union jet fuel			
JP-4			57
Saturates	NA	NA	
Olefins	NA	NA	
Aromatics	NA[**]	NA	
Jet A			57
Saturates	NA	NA	
Olefins	NA	NA	
Aromatics	NA[††]	NA	

Explanatory Notes

[*] Determined via ASTM D-1319

[†] A benzene content of 275 ppmw is reported for a petroleum-derived JP-4 in Reference 57.

[‡] Less than 1 ppmw of benzene is reported for a petroleum-derived Jet A fuel in (Reference 57).

[§] 24.9 wt. % aromatics and 75.1 wt % saturates are also reported, based on high pressure liquid chromatography results. See also Table 105.

[#] 23.5 wt. % aromatics and 76.5 wt % saturates are also reported, based on high pressure liquid chromatography results. See also Table 105.

[**] A benzene content of 331 ppmw is reported for a shale-derived JP-4 (Reference 57).

[††] A benzene content of <1 ppmw is reported for a shale-derived Jet A (Reference 57).

Table 105. Detailed Hydrocarbon Class Analysis

		Value		
Material	Compound Class	Vol. %*	Sample Description/Source	Reference
Petroleum jet fuel				
Jet A	Paraffins	40.6	API	65
	Monocycloparaffins	27.3		
	Dicycloparaffins	10.9		
	Tricycloparaffins	3.3		
	Total Saturates	82.1		
	Alkylbenzenes	10.0		
	Indans & tetralins	3.6		
	Dinaphthenobenzenes	0.9		
	C_{10} naphthalenes	0.2		
	C_{11} naphthalenes	0.1		
	Biphenyls, etc.	0.1		
	Fluorenes, etc.	0.0		
	Tricyclic aromatics	0.0		
	Total aromatics	17.9		
Shale jet fuel	Compound Class	Wt.%		
JP-5	Paraffins	46.0	Paraho-SOHIO Toledo	35
	Mononapthenes	24.3		
	Dinaphthenes	8.1		
	Total saturates	78.4		
	Alkylbenzenes	10.8		
	Indans & tetralins	10.8		
	Total aromatics	21.6†		

(Continued)

Table 105 (Concluded)

		Value		
Material	Compound Class	Vol. %[*]	Sample Description/Source	Reference
Shale jet fuel				
JP-8	Paraffins	47.0	Paraho-SOHIO Toledo	35
	Mononaphthenes	24.0		
	Dinaphthenes	7.6		
	Total saturates	78.6		
	Alkylbenzenes	11.4		
	Indans & tetralins	10.0		
	Total aromatics	21.4[‡]		

Explanatory Notes

[*] Determined by mass spectrometry via ASTM D-2425; values normalized to 100.0 volume percent.

[†] 13.54 wt% monoaromatics, 1.36 wt % diaromatics and 0.002 wt % triaromatics also reported for Paraho-SOHIO Toledo JP-5 (Reference 67).

[‡] 13.84 wt % monoaromatics, 1.19 wt% diaromatics and 0.003 wt % triaromatics also reported for Paraho-SOHIO Toledo JP-8 (Reference 67).

Table 106. Nitrogen Compound Class Analysis - Solvent Fractionation ("Type 1")*

A. Compound Type Fractions and Elemental Nitrogen Content of Fractions

Material	Nitrogen, wt. % of Fraction Hydrocarbon	Pyridine I	Pyrrole	Pyrrole/Arylamine	Pyridine II	Amide/Pyridine III	Sample Description/Source	Reference
Petroleum jet fuel	NA	NA	NA	NA	NA	NA	--	--
Shale jet fuel								
JP-8†	0.0009	7.37	8.66	8.81	8.80	7.79	Paraho - SOHIO Toledo	53

B. Potentiometric Titration Results for Compound Type Fractions

Material	Nitrogen-Type Fractions	Nitrogen, wt. % of Fraction Strong Base pKa 9 to 11	Weak Base I, pKa 7 to 9	Weak Base II, pKa 2 to 7	Weak Base II, pKa 2 to 7	Very Weak Base pKa-2 to 2	Nonbasic Nitrogen Compounds	Total	Sample Description/Source	Reference
Petroleum jet fuel	NA	NA	NA	NA	NA	NA	NA	NA	--	--
Shale jet fuel										
JP-8	Pyridine I	ND	7.13	ND	ND	0.24	ND	7.37	Paraho - SOHIO Toledo	53
	Pyrrole	ND	ND	0.18	ND	8.47	0.01	8.66		
	Pyrrole/Arylamine	ND	ND	2.10	5.40	1.31	ND	8.81		
	Pyridine II	ND	8.44	ND	ND	0.33	0.03	8.80		
	Amide/Pyridine II	0.18	3.99	ND	1.98	0.84	0.80	7.79		

(Continued)

Table 106 (Concluded)

C. Nitrogen - Compound Type Fraction Distribution

Nitrogen, wt. % of Sample

Nitrogen Compound Type	Petroleum Jet Fuel	Shale Jet Fuel Paraho - SOHIO Toledo DFM (Ref.53)
Strong Base	NA	
Alkylamines/alkylpiperidines		0.001
Weak base I	NA	
Hindered alkylpyridines/ alkylquinolines		0.121
Less hindered alkylpyridines/ alkyliquinolines/alkylacridines		0.082
Less hindered alkylpyridines/ alkylquinolines/alkylhydropyridines		0.017
Weak base II	NA	
Alkylnaphthenopiperidines		ND
Unknown		0.006
Weak base II	NA	
Alkylanilines/alkylnaphthenoanilines		0.002
Very weak base	NA	
Alkylhydroxypyridines		0.007
Alkylpyrroles/alkylindoles		0.017
Unknown		0.004
Nonbasic	NA	
N-Alkylcarbazoles		ND
Alkylpyrroles/alkylindoles/ alkylcarbazoles/alkylbenzo-carbazoles		Trace
Alkylcarboxamides/alkyldiazaaromatics		0.004
Total	NA	0.281

Explanatory Notes

*This solvent fractionation method involves separation of the sample into six compound-type fractions using basic/neutral alumina and silica adsorption chromatography; method is described in References 32 and 53.

†Original sample contained 0.30 wt. % of nitrogen; the cumulative nitrogen in the fractions is 0.281 wt. %, or 94% of the original sample.

Table 107. Nitrogen Compound Class Analysis - Solvent Fractionation ("Type 2")*

Material	Compound Class	Number of Carbons in Side Chain	Number of Isomers Detected	Relative Amount of Class	Sample Description/Source	Reference
Petroleum jet fuel	NA	NA	NA	NA	--	--
Shale jet fuel						
JP-5†	Pyridines ($C_nH_{2n-5}N$)	3	1		Paraho-SOHIO	64
		4	4		Toledo	
		5	9			
		6	10			
		7	8	85%		
		8	11			
		9	3			
		10	3			
	Tetrahydroquinolines ($C_nH_{2n-7}N$)	1	3			
		2	5			
		3	4	10%		
		4	1			
		5	2			
	Quinolines ($C_nH_{2n-11}N$)	1	1			
		2	4			
		3	3	5%		
		4	2			
		5	1			
JP-5	Pyridines‡ ($C_nH_{2n-5}N$)	2	1	NA	Paraho-SOHIO	75
		3	4	NA	Gary Western	
		4	4	NA		
		5	1	NA		
		6	5	NA		
		7	NA	NA		
		8	NA	NA		
		9	NA	NA		

(Continued)

Table 107 (Concluded)

Material	Compound Class	Number of Carbons in Side Chain	Number of Isomers Detected	Relative Amount of Class	Sample Description/Source	Reference
	Tetrahydroquinolines§ ($C_nH_{2n-7}N$)	1	1	NA	Paraho-SOHIO Gary Western	75
		2	NA	NA		
		4	NA	NA		
	Quinolines# ($C_nH_{2n-11}N$)	1	1	NA		
		2	NA	NA		
		3	NA	NA		
		Other	NA	NA		

Explanatory Notes

*This solvent fractionation method involves acid extraction followed by GC-MS analysis; details of the method can be found in Reference 64.

†The average molecular weight of the pyridine class was 172; most of the compounds contained from 5 to 8 carbons in side chains. Significant amounts of $C_nH_{2n-11}N$ (quinolines) and $C_nH_{2n-7}N$ (tetrahydroquinolines) averaging 2 to 3 carbons in side chains were also detected.

‡Includes 4-ethyl, 2-methyl-ethyl-, 4-isopropyl-, 2-propyl-3-ethyl-4-methyl, 2-propyl-methyl-, 3,4-diethyl-2-propyl-methyl-, 4-butyl-, 3-propyl-4-ethyl-, 3-propyl-4-ethyl-5-methyl-, 3-ethyl-4-butyl-, 2-propyl-3-methyl-4-ethyl-, 2-butyl-4-ethyl-, 3,4-dipropyl-, and C_6 through C_9 pyridine.

§Includes methyl-tetrahydro-, ethyl-tetrahydro-, and C_2-tetrahydroquinoline.

#Includes methyl quinoline and C_2-, C_3- and various other quinolines.

Table 108. Mercaptan Sulfur Content

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum jet fuel			
JP-4	0.0004*	Average of 20 samples	21
JP-5	0.0003*	Average of 6 samples	21
Jet A	0.0008*	Average of 54 samples	21
Shale jet fuel			
JP-4	<0.0002	Paraho-SOHIO Gary Western	38
JP-5	<0.0002	Paraho-SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-1323

General Comments

1. Additional data for Paraho-SOHIO Toledo JP-5:
   Thermal oxidation stability, JFTOT at 260°C - TDR Spun, 2.0 and TDR spot, 8.0; visual tube rating. Visual appearance, white/clear; color (ASTM rating), <0.5; accelerated stability (mg/100 ml), 0.14 (Reference 67).

2. Additional data for Paraho-SOHIO Toledo JP-8:
   Thermal oxidation stability, JFTOT at 260°C - TDR Spun, 10.0; TDR spot, 12.0; visual tube rating, 2. Visual appearance, straw/clear; color (ASTM rating), 0.5; accelerated stability (mg/100 ml), 0.29 (Reference 67).

3. The average luminometer number of 10 samples of petroleum-derived jet A fuel was 49 (Reference 21).

4. Additional data for Paraho-SOHIO Toledo jet fuel: particulate matter content, 0.1 wt % for JP-5 and 0.3 wt % for JP-8 (Reference 67).

5. Although detailed individual compound or compound class data are not available for jet fuels, hydrocarbon compound classes and individual hydrocarbon compounds found in light and medium boiling (i.e., less than 550-660°F) petroleum or shale oil distillation fractions (see data presented in Tables 22 through 27) may be present in jet fuel to various degrees, depending on the nature of the refining (e.g., blending) practices used.

6. Although no individual PNA compound data are available for jet fuels, based on the limited quantitative data on triaromatics content presented in Table 105, and the fact that various tetraaromatics and higher boiling compounds have been found in the lower and medium boiling fractions of petroleum crudes and hydrotreated shale oils (see Table 36), very low levels of certain PNA's are likely to be present in petroleum- and shale-derived jet fuels.

7. The following basic nitrogen values were reported for Paraho-SOHIO Gary Western jet fuels: (a) 115 ppm for JP-4; (b) 895 ppm for JP-5 (Reference 38).

8. Detailed data are unavailable on individual sulfur- and oxygen-containing compounds or compound classes in petroleum- and shale-derived jet fuel.

Part IV. Diesel Fuel

Table 109. Specific Gravity

Material	Value	Sample Description/Source	Reference
Petroleum diesel			
No. 2 fuel oil	0.85	NA	15
Shale diesel			
DFM/DF-2	0.8612	Paraho - SOHIO Gary Western	38
DFM	0.8353	Paraho - SOHIO Toledo	67
City bus diesel	0.8159*	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	0.8262*	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	0.8300*	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	0.8367*	In-situ; Rock Springs, WY - LETC	46

Explanatory Notes

*Determined at 60/60°F

Table 110. API Gravity

Material	Value (°)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	43.2*	Average of 34 Eastern region samples	22
	42.4*	Average of 15 Southern region samples	22
	42.5*	Average of 33 Central region samples	22
	42.1*	Average of 16 Rocky Mtn. region samples	22
	42.8*	Average of 17 Western region samples	22
Grade 2 heating oil	35.2*	Average of 54 Eastern region samples	22
	35.2*	Average of 26 Southern region samples	22
	35.3*	Average of 40 Central region samples	22
	35.6*	Average of 23 Rocky Mtn. region samples	22
	36.2*	Average of 21 Western region samples	22
	35.5†	API No. 78-2	70
	35.7†	API No. 78-3	70
	36.2†	API No. 78-4	70
	36.2†	API No. 79-4	70
City bus diesel	33.3 - 47.2	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	27.3 - 47.4	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	9.6 - 41.1	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	27.2 - 43.4	Range of U.S. diesel fuels produced in 1974	46
No. 2 fuel oil	35	NA	15
Shale diesel			
DFM	38.1	Paraho - SOHIO Toledo	33
	37.9	Paraho - SOHIO Toledo	67
DFM/DF-2	32.8	Paraho - SOHIO Gary Western	38
City bus diesel	41.93	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	39.75	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	38.98	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	37.62	In-situ; Rock Springs, WY - LETC	46

Explanatory Notes

*Determined via ASTM D-287

†Determined via ASTM D-1298

Table 111. Viscosity

Material	Value (centistokes)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	1.62*	Average of 34 Eastern region samples	22
	1.62*	Average of 15 Southern region samples	22
	1.67*	Average of 33 Central region samples	22
	1.69*	Average of 16 Rocky Mtn. region samples	22
	1.58*	Average of 17 Western region samples	22
Grade 2 heating oil	2.67*	Average of 54 Eastern region samples	22
	2.70*	Average of 26 Southern region samples	22
	2.52*	Average of 40 Central region samples	22
	2.72*	Average of 23 Rocky Mtn. region samples	22
	2.80*	Average of 21 Western region samples	22
	3.2*	API No. 78-2	70
	3.5*	API No. 78-3	70
	2.6*	API No. 78-4	70
	2.6*	API No. 79-4	70
City bus diesel	1.50 - 4.34	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	1.30 - 4.55	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine	1.94 - 4.34	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	1.60 - 22.1	Range of U.S. diesel fuels produced in 1974	46
Diesel fuel	2.4	API No. 2-DA	69
	2.17	API No. 79-6	68
No. 2 fuel oil	34-40 SSU (100°F)	NA	15
Shale diesel			
DFM	2.599	Paraho - SOHIO Toledo	35
	2.71	Paraho - SOHIO Toledo	67
DFM/DF-2	5.54†	Paraho - SOHIO Gary Western	38
City bus diesel	1.66†	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	2.40†	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	2.96†	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	5.07	In-situ; Rock Springs, WY - LETC	46

Explanatory Notes

*Determined via ASTM D-445 at 100°F

†Measured at 100°F

Table 112. Pour Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	<-70 to <-20*	Range of 34 Eastern region samples	22
	<-70 to <-40*	Range of 15 Southern region samples	22
	<-60 to -25*	Range of 33 Central region samples	22
	-80 to -30*	Range of 16 Rocky Mtn. region samples	22
	-80 to <-25*	Range of 17 Western region samples	22
Grade 2 heating oil	-50 to 5*	Range of 54 Eastern region samples	22
	-50 to 5*	Range of 26 Southern region samples	22
	-40 to 10*	Range of 40 Central region samples	22
	-60 to 10*	Range of 23 Rocky Mtn. region samples	22
	-60 to 20*	Range of 21 Western region samples	22
	-10*	API No. 78-2	70
	-10*	API No. 78-3	70
	-10*	API No. 78-4	70
	-10*	API No. 79-4	70
City bus diesel	-70 to 25	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	<-60 to 25	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	-35 to 65	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	-40 to 25	Range of U.S. diesel fuels produced in 1974	46
No. 2 fuel oil	0	NA	15
Shale diesel			
DFM	<-5*	Paraho - SOHIO Toledo	35
	-5.8*	Paraho - SOHIO Toledo	57
	-0.4	Paraho - SOHIO Toledo	67
DFM/DF-2	50	Paraho - SOHIO Gary Western	38
City bus diesel	-50	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	-30	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	-20	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	30	In-situ; Rock Springs, WY - LETC	46
	-27.4	NA	57

Explanatory Notes

*Determined via ASTM D-97

Table 113. Carbon Residue

Material	Value (wt %)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	0.052*	Average of 34 Eastern region samples	22
	0.049*	Average of 15 Southern region samples	22
	0.060*	Average of 33 Central region samples	22
	0.054*	Average of 16 Rocky Mtn. region samples	22
	0.064*	Average of 17 Western region samples	22
Grade 2 heating oil	0.103*	Average of 54 Eastern region samples	22
	0.104*	Average of 26 Southern region samples	22
	0.120*	Average of 40 Central region samples	22
	0.104*	Average of 23 Rocky Mtn. region samples	22
	0.093*	Average of 21 Western region samples	22
	0.07‡	API No. 78-2	70
	0.08‡	API No. 78-3	70
	0.13‡	API No. 78-4	70
	0.13‡	API No. 79-4	70
City bus diesel	0.000 - 0.18§	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	0.001 - 0.26§	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	0.014 - 0.26§	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	0.05 - 0.18§	Range of U.S. diesel fuels produced in 1974	46
Shale diesel			
DFM/DF-2	1.21†, 0.60‡	Paraho - SOHIO Gary Western	38
City bus diesel	0.14§	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	0.16§	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	0.36§	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	0.42§	In-situ; Rock Springs, WY - LETC	46

Explanatory Notes

*Determined via ASTM D-524

†Conradson carbon number

‡Ramsbottom carbon number

§Carbon residue on 10 percent bottoms

Table 114. Density

Material	Value (g/ml)*	Sample Description/Source	Reference
Petroleum diesel			
diesel fuel	0.8784	E. Wilmington, CA crude	57
Shale diesel			
DFM	0.8342	Paraho - SOHIO Toledo	57
	0.8261	NA	57

Explanatory Notes

*Determined via ASTM D-1481 at 60°F

Table 115. Reid Vapor Pressure

Material	Value	Sample Description/Source	Reference
Petroleum diesel	NA	--	--
Shale diesel	<0.1 psi	NA	57

Table 116. Distillation Data

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	349°F - IBP 381°F - 10 424°F - 50 476°F - 90 518°F - EP	Average of 34 Eastern region samples	22
	350°F - IBP 381°F - 10 420°F - 50 476°F - 90 520°F - EP	Average of 15 Southern region samples	22
	347°F - IBP 381°F - 10 427°F - 50 485°F - 90 425°F - EP	Average of 33 Central region samples	22
	342°F - IBP 381°F - 10 430°F - 50 491°F - 90 532°F - EP	Average of 16 Rocky Mtn. region samples	22
	338°F - IBP 378°F - 10 422°F - 50 478°F - 90 518°F - EP	Average of 17 Western region samples	22

(Continued)

Table 116 (Continued)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum diesel			
Grade 2 heating oil	366°F - IBP 421°F - 10 501°F - 50 595°F - 90 645°F - EP	Average of 54 Eastern region samples	22
	372°F - IBP 425°F - 10 506°F - 50 601°F - 90 647°F - EP	Average of 26 Southern region samples	22
	368°F - IBP 417°F - 10 497°F - 50 585°F - 90 638°F - EP	Average of 40 Central region samples	22
	374°F - IBP 428°F - 10 500°F - 50 585°F - 90 635°F - EP	Average of 23 Rocky Mtn. region samples	22
	383°F - IBP 439°F - 10 504°F - 50 585°F - 90 634°F - EP	Average of 21 Western region samples	22

(Continued)

Table 116 (Continued)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum diesel			
Grade 2 heating oil	NA - IBP 486°F - 10 533°F - 50 581°F - 90 624°F - EP	API No. 78-2	70
	NA - IBP 479°F - 10 542°F - 50 580°F - 90 628°F - EP	API No. 78-3	70
	437°F - IBP 470°F - 10 511°F - 50 572°F - 90 610°F - EP	API No. 78-4	70
	437°F - IBP 470°F - 10 511°F - 50 572°F - 90 610°F - EP	API No. 79-4	70
City bus diesel	320-488°F - IBP 357-520°F - 10 403-558°F - 50 454-603°F - 90 476-663°F - EP	Range of U.S. diesel fuels produced in 1974	46

(Continued)

Table 116 (Continued)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum diesel			
Truck-tractor diesel	301-488°F - IBP 329-520°F - 10 382-596°F - 50 444-656°F - 90 476-700°F - EP	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	327-535°F - IBP 384-595°F - 10 454-680°F - 50 535-656°F - 90 582-700°F - EP	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	310-488°F - IBP 376-520°F - 10 434-558°F - 50 476-639°F - 90 514-688°F - EP	Range of U.S. diesel fuels produced in 1974	46
Diesel fuel	372°F - IBP 405°F - 5 418°F - 10 437°F - 20 453°F - 30 471°F - 40 490°F - 50 512°F - 60 538°F - 70 565°F - 80 605°F - 90 636°F - 95 656°F - EP	API No. 2 - DA	69

(Continued)

Table 116 (Continued)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Petroleum diesel			
Diesel fuel (Continued)	367°F - IBP	API No. 79-6	68
	412°F - 5		
	428°F - 10		
	457°F - 20		
	478°F - 30		
	489°F - 40		
	512°F - 50		
	529°F - 60		
	554°F - 70		
	578°F - 80		
	615°F - 90		
	648°F - 95		
	675°F - EP		
No. 2 fuel oil	430°F - IBP	NA	15
	625°F - 90		
	675°F - EP		
Shale diesel			
DFM	403°F - IBP	Paraho - SOHIO Toledo	67
	451°F - 10		
	469°F - 20		
	507°F - 50		
	563°F - 90		
	594°F - EP†		

(Continued)

Table 116 (Continued)

Material	Value (% Evaporation)	Sample Description/Source	Reference
City bus diesel	379°F - IBP	In-situ; Rock Springs, WY-LETC	46
	400°F - 10		
	409°F - 20		
	414°F - 30		
	418°F - 40		
	422°F - 50		
	429°F - 60		
	437°F - 70		
	447°F - 80		
	469°F - 90		
	517°F - EP‡		
Shale diesel			
Truck-tractor diesel	404°F - IBP	In-situ; Rock Springs, WY-LETC	46
	442°F - 10		
	454°F - 20		
	465°F - 30		
	474°F - 40		
	484°F - 50		
	494°F - 60		
	505°F - 70		
	518°F - 80		
	537°F - 90		
	554°F - EP§		

(Continued)

Table 116 (Concluded)

Material	Value (% Evaporation)	Sample Description/Source	Reference
Stationary-marine diesel	410°F - IBP 450°F - 10 468°F - 20 483°F - 30 495°F - 40 507°F - 50 524°F - 60 546°F - 70 573°F - 80 605°F - 90 628°F - EP#	In-situ; Rock Springs, WY-LETC	46
Shale diesel			
No. 4 fuel oil	394°F - IBP 528°F - 10 562°F - 20 572°F - 30 580°F - 40 588°F - 50 599°F - 60 610°F - 70 624°F - 80 666°F - 90 667°F - EP**	In-situ; Rock Springs, WY-LETC	46

Explanatory Notes

*Determined by ASTM D-86

†Recovery, 99%; residue, 1%; loss, 0%

‡Recovery, 95.0 vol %; residue, 2.0 vol %; loss, 3.0 vol %

§Recovery, 98.0 vol %; residue, 1.0 vol %; loss, 1.0 vol %

#Recovery, 97.5 vol %; residue, 2.0 vol %; loss, 0.5 vol %

**Recovery, 92.0 vol %; residue, 7.0 vol %; loss, 1.0 vol %

Table 117. GC Simulated Distillation Data*

Material	Building Point Range (°C)	Sample Description/Source	Reference
Petroleum diesel			
Diesel fuel	5% recovered - 175	E. Wilmington, CA crude	57
	50% recovered - 273		
	95% recovered - 349		
Shale diesel			
DFM	5% recovered - 192	Paraho - SOHIO Toledo	57
	50% recovered - 268		
	95% recovered - 322		
	0.1% recovered - 217	Paraho - SOHIO Toledo	67
	1% recovered - 306		
	10% recovered - 417		
	20% recovered - 457		
	50% recovered - 520		
	90% recovered - 601		
	95% recovered - 613		
	99% recovered - 637		
	99.5% recovered - 678		
	5% recovered - 174	NA	57
	50% recovered - 269		
	95% recovered - 353		

Explanatory Note

*GC simulated distillation involves use of gas chromatograph rather than distillation column. Retention times of sample peaks are based on retention times of a calibration mixture of C_3 to C_{42} normal paraffins. The boiling range distribution of the sample is calculated in weight percent via computer. Volume percent values are calculated from a density - boiling point correlation of normal paraffins (Reference 35).

Table 118. Refractive Index

Material	Value (Abbe refractometer, 67°C)	Sample Description/Source	Reference
Petroleum diesel	NA	--	--
Shale diesel DFM	1.4471	Paraho - SOHIO Toledo	35

Table 119. Molecular Weight (Cryoscopic)

Material	Value	Sample Description/Source	Reference
Petroleum diesel	NA	--	--
Shale diesel DFM	201	Paraho - SOHIO Toledo	35

Table 120. Bottom Sediment and Water

Material	Value (Vol. %)*	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	0.001*	Average of 34 Eastern region samples	22
	0.001*	Average of 15 Southern region samples	22
	0.0004*	Average of 33 Central region samples	22
	0.0001*	Average of 16 Rocky Mtn. region samples	22
	0.0001*	Average of 17 Western region samples	22
Grade 2 heating oil	0.003*	Average of 54 Eastern region samples	22
	0.002*	Average of 26 Southern region samples	22
	0.002*	Average of 40 Central region samples	22
	0.000*	Average of 23 Rocky Mtn. region samples	22
	0.003*	Average of 21 Western region samples	22
Shale diesel DFM/DF-2	0.1 (wt %)	Paraho - SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-1796

Table 121. Total Acid Number

Material	Value (mg KOH/g)	Sample Description/Source	Reference
Petroleum diesel			
Diesel fuel	1.31*	E. Wilmington, CA crude	57
	0.0*	API No. 79-6	68
Shale diesel			
DFM/DF-2	0.7	Paraho - SOHIO Gary Western	38
DFM	0.010	Paraho - SOHIO Toledo	33
	0.001	Paraho - SOHIO Toledo	67
	0.02	NA	57

Explanatory Notes

*Determined via ASTM D-974

Table 122. Flash Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	122 - 156*	Range of 34 Eastern region samples	22
	122 - 146*	Range of 15 Southern region samples	22
	118 - 150*	Range of 33 Central region samples	22
	118 - 162*	Range of 16 Rocky Mtn. region samples	22
	108 - 156*	Range of 17 Western region samples	22
Grade 2 heating oil	126 - 200*	Range of 54 Eastern region samples	22
	126 - 176*	Range of 26 Southern region samples	22
	126 - 192*	Range of 40 Central region samples	22
	138 - 206*	Range of 23 Rocky Mtn. region samples	22
	134 - 204*	Range of 21 Western region samples	22
City bus diesel	124 - 194	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	112 - 230	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	136 - 290	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	136 - 198	Range of U.S. diesel fuels produced in 1974	46
Diesel fuel	136* 142*	API No. 2-DA API No. 79-6	69 68

(Continued)

Table 122 (Concluded)

Material	Value (°F)	Sample Description/Source	Reference
Shale diesel			
DFM/DF-2	168	Paraho - SOHIO Gary Western	38
DFM	176	Paraho - SOHIO Toledo	67
City bus diesel	188	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	212	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	265	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	325	In-situ; Rock Springs, WY - LETC	46

Explanatory Notes

*Determined via ASTM D-56

Table 123. Cloud Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum diesel			
Diesel fuel	-32.8	E. Wilmington, CA crude	57
Grade 1 heating oil	-66 to -20*	Range of 34 Eastern region samples	22
	-66 to -36*	Range of 15 Southern region samples	22
	-58 to -20*	Range of 33 Central region samples	22
	-60 to -20*	Range of 16 Rocky Mtn. region samples	22
	-60 to <-20*	Range of 17 Western region samples	22
Grade 2 heating oil	-22 to 20*	Range of 54 Eastern region samples	22
	- 6 to 12*	Range of 26 Southern region samples	22
	-10 to 12*	Range of 40 Central region samples	22
	-54 to 22*	Range of 23 Rocky Mtn. region samples	22
	-54 to 42*	Range of 21 Western region samples	22
No. 2 fuel oil	10	NA	15
Shale diesel			
DFM/DF-2	--(too dark to see)	Paraho - SOHIO Gary Western	38
DFM	50	Paraho - SOHIO Toledo	67
	-0.4	NA	57

Explanatory Notes

*Determined via ASTM D-2500

Table 124. Aniline Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum diesel			
Grade 1 heating oil	145.8*	Average of 34 Eastern region samples	22
	143.0*	Average of 15 Southern region samples	22
	144.6*	Average of 33 Central region samples	22
	143.9*	Average of 16 Rocky Mtn. region samples	22
	140.9*	Average of 17 Western region samples	22
Grade 2 heating oil	142.1*	Average of 54 Eastern region samples	22
	145.9*	Average of 26 Southern region samples	22
	141.3*	Average of 40 Central region samples	22
	144.7*	Average of 23 Rocky Mtn. region samples	22
	147.9*	Average of 21 Western region samples	22
Shale diesel			
DFM/DF-2	120.2	Paraho - SOHIO Gary Western	38
DFM	153	Paraho - SOHIO Toledo	67

Explanatory Notes

*Determined via ASTM D-611

Table 125. Heat of Combustion

Material	Value (Net Btu/lb)	Sample Description/Source	Reference
Petroleum diesel			
No. 2 fuel oil	19,840	NA	9
	18,330	NA	15
Shale diesel			
DFM/DF-2	17,962*	Paraho - SOHIO Gary Western	38
DFM	18,284	Paraho - SOHIO Toledo	67

Explanatory Notes

*Gross heat of combustion is 18,974 Btu/lb.

Table 125. Heat of Combustion

Material	Value (Net Btu/lb)	Sample Description/Source	Reference
Petroleum diesel			
No. 2 fuel oil	19,840	NA	9
	18,330	NA	15
Shale diesel			
DFM/DF-2	17,962*	Paraho - SOHIO Gary Western	38
DFM	18,284	Paraho - SOHIO Toledo	67

Explanatory Notes

*Gross heat of combustion is 18,974 Btu/lb.

Table 126. Corrosion Rating

Material	Value	Sample Description/Source	Reference
Petroleum diesel		--	--
No. 2 home heating oil	1A*	API No. 78.2	70
	1A*	API No. 78-3	70
	1A*	API No. 78-4	70
	1A*	API No. 79-4	70
Shale diesel			
DFM/DF-2	1A at 3 hr/212°F	SOHIO Gary Western	38
DFM	1A	SOHIO Toledo	67

Explanatory Notes

*Determined using copper strip method for 3 hours at 122°F.

Table 127. Cetane Index

Material	Value	Sample Description/Source	Reference
Petroleum diesel			
City bus diesel	39.8 - 65.8	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	38.1 - 65.8	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	38.0 - 63.1	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	34.1 - 65.8	Range of U.S. diesel fuels produced in 1974	46
No. 2 fuel oil	42 - 43	NA	15
Shale diesel			
DFM	50.1 49	Paraho - SOHIO Toledo Paraho - SOHIO Toledo	33 67
DFM/DF-2	57.3	Paraho - SOHIO Gary Western	38
City bus diesel	48	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	54	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	56	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	65	In-situ; Rock Springs, WY - LETC	46

Table 128. Oxygen Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum diesel			
Diesel fuel	0.36	E. Wilmington, CA crude	57
Shale diesel			
DFM	0.37	Paraho - SOHIO Toledo	67
	0.008	Paraho - SOHIO Toledo	35
	0.024	NA	57

Table 129. Sulfur Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum Diesel			
Diesel fuel	0.89	E. Wilmington, CA crude	57
	0.1	API No. 2-DA	69
	0.19	API No. 79-6	68
No. 2 fuel oil	0.21	NA	9
	0.035 - 0.45	NA	15
Grade 1 heating oil	0.065*	Average of 34 Eastern region samples	22
	0.039*	Average of 15 Southern region samples	22
	0.078*	Average of 33 Central region samples	22
	0.090*	Average of 16 Rocky Mtn. region samples	22
	0.079*	Average of 17 Western region samples	22
Grade 2 heating oil	0.245*	Average of 54 Eastern region samples	22
	0.201*	Average of 26 Southern region samples	22
	0.263*	Average of 40 Central region samples	22
	0.261*	Average of 23 Rocky Mtn. region samples	22
	0.240*	Average of 21 Western region samples	22

(Continued)

Table 129 (Concluded)

Material	Value (Wt. %)	Sample Description/Source	Reference
City bus diesel	0.004 - 0.52	Range of U.S. diesel fuels produced in 1974	46
Truck-tractor diesel	0.001 - 1.07	Range of U.S. diesel fuels produced in 1974	46
Stationary-marine diesel	0.06 - 2.85	Range of U.S. diesel fuels produced in 1974	46
Railroad diesel	0.01 -0.85	Range of U.S. diesel fuels produced in 1974	46
Shale diesel			
DFM	0.0007	Paraho - SOHIO Toledo	35
	0.004	Paraho - SOHIO Toledo	67
DFM/DF-2	0.44	Paraho - SOHIO Gary Western	38
City bus diesel	0.01	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	0.02	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	0.02	In-situ; Rock Springs, WY - LETC	46
No. 4 fuel oil	0.02	In-situ; Rock Springs, WY - LETC	46

Explatory Notes

*Determined via ASTM D-129

Table 130. Nitrogen Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum diesel			
Diesel fuel	0.056	E. Wilmington, CA crude	57
Shale diesel			
DFM	<0.0001	Paraho - SOHIO Toledo	67
	0.0015	Paraho - SOHIO Toledo	35
	0.00039	Paraho - SOHIO Toledo	33
	0.0021	NA	57
DFM/DF-2	0.233	Paraho - SOHIO Gary Western	38
City bus diesel	0.0141	In-situ Rock; Springs, WY - LETC	46
Truck-tractor diesel	0.0166	In-situ Rock; Springs, WY - LETC	46
Stationary-marine diesel	0.0202	In-situ Rock; Springs, WY - LETC	46
Railroad diesel	0.0396	In-situ Rock; Springs, WY - LETC	46

Table 131. Carbon Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum diesel			
No. 2 fuel oil	87.3	NA	9
Shale diesel			
DFM	86.54	Paraho - SOHIO Toledo	67
	86.6	Paraho - SOHIO Toledo	35
	86.27	Paraho - SOHIO Toledo	33

Table 131. Carbon Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum diesel			
No. 2 fuel oil	87.3	NA	9
Shale diesel			
DFM	86.54	Paraho - SOHIO Toledo	67
	86.6	Paraho - SOHIO Toledo	35
	86.27	Paraho - SOHIO Toledo	33

Table 132. Hydrogen Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum diesel			
No. 2 fuel oil	12.5	NA	9
Shale diesel			
DFM	13.36	Paraho - SOHIO Toledo	67
	13.4	Paraho - SOHIO Toledo	35
	13.28	Paraho - SOHIO Toledo	33

Table 133. Trace Elements Content (ppmw)*

Material	Al	Sb	As	Be	Cd	Ca	Cl	Co	Cr	Cu
Petroleum diesel										
Diesel fuel	NA	<0.5	0.3	NA	<0.03	NA	NA	NA	<0.05	<0.05
Diesel fuel	NA	NA	0.012 0.13	NA	0.089 - 0.89	NA	NA	NA	0.55 - 2.8	NA
Shale diesel										
DFM	0.047 (NAA)	ND(<3) (XRF)	ND(<0.5) (XRF)	<0.01 (AA)	<0.02 (AA)	ND(≤0.6) (NAA)	ND(<2) (XRF)	<0.06 (FE)	ND(≤0.047) (NAA)	<0.02 (AA)
	NA	<0.5	1.4	NA	<0.03	NA	NA	NA	<0.05	<0.05

Material	Fe	Pb	Mg	Mn	Hg	Mo	Ni	Se	Si	Ag	Na
Petroleum diesel											
Diesel fuel	<0.05	0.07	NA	NA	<1	NA	<0.05	<0.3	NA	NA	NA
Diesel fuel	3.8 - 71.0	<0.49 - 2.0	NA	0.29 6.2	NA	0.018 - 0.27	<6.1 - 23.0	NA	NA	NA	NA
Shale diesel											
DFM	<0.01 (FE)	<0.06 (AA)	ND(≤5.3) (NAA)	<0.02 (AA)	ND(≤2.0) (XRF)	ND(≤0.019) (NAA)	ND(≤2.4) (NAA)	ND(≤0.5) (XRF)	ND(≤10) (NAA)	<0.02 (AA)	0.16(FE)
	<0.05	<0.06	NA	NA	3†	NA	<0.05	<0.3	NA	NA	NA

(Continued)

Table 133 (Concluded)

Material	Sr	Th	Sn	Tl	V	Zn	Sample Description/Source	Reference
Petroleum diesel								
Diesel fuel	NA	NA	NA	NA	<0.05	<0.05	E. Wilmington, CA crude	57
Diesel fuel	NA	NA	NA	NA	<0.05 - 0.16	1.3 - 4.8	Range of 6 domestic diesel fuels	24
Shale diesel								
DFH	ND(≤0.75) (NAA)	ND(<6.0) (XRF)	ND(≤0.57) (NAA)	ND(<0.4) (XRF)	ND(<0.0008) (NAA)	<0.02 (AA)	Paraho - SOHIO Toledo	35
	NA	NA	NA	NA	<0.05	<0.05	NA	57

Explanatory Notes

*Methods used include atomic absorption spectroscopy (AA), flame emission spectroscopy (FE), neutron activation analysis (NAA), and X-ray fluorescence (XRF).

†Result may be an artifact of laboratory processing, since no mercury was detected in the raw shale oil.

Table 134. Ash Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum diesel			
City bus diesel	0.000 - 0.005	Range of U.S. diesel fuels produced during 1974	46
Truck-tractor diesel	0.000 - 0.010	Range of U.S. diesel fuels produced during 1974	46
Stationary-marine diesel	0.000 - 0.02	Range of U.S. diesel fuels produced during 1974	46
Railroad diesel	0.000 - 0.005	Range of U.S. diesel fuels produced during 1974	46
No. 2 fuel oil	0.02	NA	15
Shale diesel			
DFM	0	Paraho - SOHIO Toledo	67
DFM/DF-2	0.0000	Paraho - SOHIO Gary Western	38
City bus diesel	<0.001	In-situ; Rock Springs, WY - LETC	46
Truck-tractor diesel	<0.001	In-situ; Rock Springs, WY - LETC	46
Stationary-marine diesel	<0.001	In-situ; Rock Springs, WY - LETC	46
Railroad diesel	<0.001	In-situ; Rock Springs, WY - LETC	46

Table 135. Saturates, Olefins and Aromatic Contents*

Material	Value (Vol. %)	Sample Description/Source	Reference
Petroleum diesel	NA[†]	--	--
Shale diesel			
DFM			
Saturates[‡]	NA	Paraho - SOHIO Toledo	67
Olefins	1		
Aromatics[†,§]	30		
Saturates	71.0	Paraho - SOHIO Toledo	33
Olefins	0.00		
Aromatics	29.0		
DFM/DF-2			
Saturates	59.6	Paraho - SOHIO Gary Western	38
Olefins	11.5		
Aromatics	25.3		
Other	3.6		

Explanatory Notes

*See also Table 136.

[†] A benzene content of 4 ppmv is reported for a petroleum-derived diesel fuel in Reference 57; a description of sample source is not provided.

[‡] Weight %'s saturates and aromatics, determined by high performance liquid chromatography, are 72.2 and 27.8, respectively.

[§] Weight % mono-, di- and triaromatics are 11.58, 4.03 and 0.045, respectively.

Table 136. Detailed Hydrocarbon Class Analysis

	Value*			
Material	Compound Class	Wt %	Sample Description/Source	Reference
Petroleum diesel	Paraffins	42.7	API No. 2-DA	69
	Cycloparaffins			
	Mono	23.4		
	Di	8.0		
	Tri	2.0		
	Total	33.4		
	Aromatics			
	Alkylbenzenes	9.7		
	Indans + tetralins	4.8		
	Dinaphthenobenzenes	1.3		
	Alkylnaphthalenes	5.3		
	Biphenyls, etc.	1.3		
	Fluorenes, etc.	0.7		
	Tricyclic aromatics	0.8		
	Benzene	47 ppm v/v		
	Total	23.9		
	Paraffins	41.7	API No. 79-6	68
	Cycloparaffins	18.8		
	Mono	9.3		
	Di	2.8		
	Tri			
	Total	30.9		
	Aromatics			
	Alkylbenzenes	8.4		
	Indans + tetralins	5.3		
	Dinaphthenobenzenes	1.1		
	C_{11} + Naphthalenes	7.6		
	Biphenyls, etc.	2.5		
	Fluorenes, etc.	1.1		
	Tricyclic aromatics	1.4		
	Total	27.4		

(Continued)

Table 136. Detailed Hydrocarbon Class Analysis

	Value*			
Material	Compound Class	Wt %	Sample Description/Source	Reference
Petroleum diesel	Paraffins	42.7	API No. 2-DA	69
	Cycloparaffins			
	Mono	23.4		
	Di	8.0		
	Tri	2.0		
	Total	33.4		
	Aromatics			
	Alkylbenzenes	9.7		
	Indans + tetralins	4.8		
	Dinaphthenobenzenes	1.3		
	Alkylnaphthalenes	5.3		
	Biphenyls, etc.	1.3		
	Fluorenes, etc.	0.7		
	Tricyclic aromatics	0.8		
	Benzene	47 ppm v/v		
	Total	23.9		
	Paraffins	41.7	API No. 79-6	68
	Cycloparaffins	18.8		
	Mono	9.3		
	Di	2.8		
	Tri			
	Total	30.9		
	Aromatics			
	Alkylbenzenes	8.4		
	Indans + tetralins	5.3		
	Dinaphthenobenzenes	1.1		
	C_{11} + Naphthalenes	7.6		
	Biphenyls, etc.	2.5		
	Fluorenes, etc.	1.1		
	Tricyclic aromatics	1.4		
	Total	27.4		

(Continued)

Table 136 (Concluded)

Material	Value* Compound Class	 Wt %	Sample Description/Source	Reference
Shale diesel DFM	Paraffins	42.8	Paraho - SOHIO Toledo	35
	Mononaphthenes	18.2		
	Polynapthenes	10.8		
	Total Saturates	71.8		
	Alkylbenzenes	8.1		
	Indans + tetralins	11.3		
	Dinaphthenobenzenes	4.6		
	Total monoaromatics	24.0		
	Naphthalenes	1.9		
	Biphenyls	1.2		
	Fluorenes	0.8		
	Total diaromatics	3.9		
	Phenanthrenes	0.3		
	Total triaromatics	0.3		
	Total aromatics	28.2		

Explanatory Notes

*Petroleum diesel data determined by mass spectrometry via ASTM D-975.

Table 137. Detailed PNA Composition

Material	Value* Compound Class	 µg/g	Sample Description/Source	Reference
Petroleum diesel	NA	NA	--	--
Shale diesel DFM	Fluorene	124		31
	Phenanthrene	281		
	Anthracene	<10		
	Fluoranthene	< 1		
	Pyrene	< 1		
	Benz(a)anthracene	< 1		
	Chrysene	< 1		
	Triphenylene	< 1		
	Me-B(a)A	< 1		
	DMe/Et-B(a)A	< 1		
	Benzo(g,h,i)fluoranthene	< 1		
	Benzo(b)fluoranthene	< 1		
	Benzo(j)fluoranthene	< 1		
	Benzo(k)fluoranthene	< 1		
	Perylene	< 1		
	Benzo(e)pyrene	< 1		
	Benzo(a)pyrene	< 1		
	Methyl B(e)P	< 1		
	Methyl B(a)P	< 1		
	1,2,3 Indeno (c,d)pyrene	< 1		
	Dibenz(a,h)anthracene	< 1		
	Benzo(g,h,i)perylene	< 1		
	Coronene	< 1		

Explanatory Notes

*Determined by GC/UV method

Table 138. Nitrogen Compound Class Analysis - Solvent Fractionation ("Type 1")*

A. Compound Type Fractions and Elemental Nitrogen Content of Fractions

	Nitrogen, wt. % of Fraction							
Material	Hydrocarbon	Pyridine I	Pyrrole	Pyrrole/Arylamine	Pyridine II	Amide/Pyridine III	Sample Description/Source	Reference
Petroleum diesel	NA	NA	NA	NA	NA	NA	--	--
Shale diesel								
DFN[†]	0.0002	6.53	7.82	8.21	7.31	7.38	Paraho - SOHIO Toledo	53

B. Potentiometric Titration Results for Compound Type Fractions

		Nitrogen, wt. % of Fraction								
Material	Nitrogen Type Fractions	Strong Base pKa 9 to 11	Weak Base I, pKa 7 to 9	Weak Base II, pKa 2 to 7	Weak Base II, pKa 2 to 7	Very Weak Base pKa-2 to 2	Nonbasic Nitrogen Compounds	Total	Sample Description/Source	Reference
Petroleum diesel	--	NA	NA	NA	NA	NA	NA	NA	--	--
Shale diesel										
DFN	Pyridine I	ND	6.04	ND	ND	0.49	ND	6.53	Paraho - SOHIO Toledo	53
	Pyrrole	ND	ND	ND	ND	4.66	3.16	7.82		
	Pyrrole/Arylamine	ND	ND	2.02	4.85	1.34	ND	8.21		
	Pyridine II	ND	6.68	ND	ND	0.44	0.19	7.31		
	Amide/Pyridine II	0.20	4.55	0.86	ND	1.77	ND	7.38		

Table 138 (Concluded)

C. Nitrogen - Compound Type Fraction Distribution

Nitrogen Compound Type	Nitrogen, wt. % of Sample Petroleum Diesel	Shale Diesel Paraho - SOHIO Toledo DFM (Ref. 53)
Strong Base	NA	
Alkylamines/alkylpiperidines		0.001
Weak base I	NA	
Hindered alkylpyridines/ alkylquinolines		0.124
Less hindered alkylpyridines/ alkyliquinolines/alkylacridines		0.063
Less hindered alkylpyridines/ alkylquinolines/alkylhydropyridines		0.016
Weak base II	NA	
Alkylnaphthenopiperidines		0.003
Unknown		0.006
Weak base II	NA	
Alkylanilines/alkylnaphthenoanilines		0.015
Very weak base	NA	
Alkylhydroxypyridines		0.010
Alkylpyrroles/alkylindoles		0.030
Unknown		0.010
Nonbasic	NA	
N-Alkylcarbazoles		ND
Alkylpyrroles/alkylindoles/ alkylcarbazoles/alkylbenzo- carbazoles		0.018
Alkylcarboxamides/alkyldiazaaromatics		0.002
Total	NA	0.298

Explanatory Notes

*This solvent fractionation method involves separation of the sample into six compound-type fractions using basic/neutral alumina and silica adsorption chromatography; method is described in References 32 and 53.

†Original sample contained 0.33 wt. % of nitrogen; the cumulative nitrogen in the fractions is 0.298 wt. %, or 90% of the original sample.

Table 139. Nitrogen Compound Class Analysis - Solvent Fractionation ("Type 2")*

Material	Compound Class	Number of Carbons in Side Chain	Number of Isomers Detected	Relative Amount Of Class	Sample Description/Source	Reference
Petroleum diesel	--	NA	NA	NA	--	--
Shale diesel					Paraho - SOHIO Toledo	64
DFM[†],[‡]	Pyridines ($C_nH_{2n-5}N$)	3	1	64%		
		4	3			
		5	7			
		6	6			
		7	14			
		8	5			
		9	6			
		10	9			
		11	3			
		12	13			
	Tetrahydro-quinolines ($C_nH_{2n-7}N$)	2	5	8%		
		3	2			
		4	4			
		5	0			
		6	2			
	Indoles ($C_nH_{2n-9}N$)	4	2	21%		
		5	2			
		6	3			
		7	8			
		8	9			
	Quinolines ($C_nH_{2n-11}N$)	2	1	7%		
		3	2			
		4	2			
		5	2			
		6	1			

Explanatory Notes

*This solvent fractionation method involves acid extraction followed by GC-MS analysis; details of the method can be found in Reference 64.

[†] Over 100 nitrogen-containing compounds were detected; the average molecular weight was 195. The indole-type compounds were primarily seven and eight carbon side chain isomers.

GENERAL COMMENTS

1. Additional data available for petroleum diesel fuel: bromine number, determined by ASTM D-1159, 0.6 for API No. 2-DA (Reference 69) and 1.42 for API No. 79-6 (Reference 68).

2. Additional data available for Paraho - SOHIO Gary Western DFM/DF-2: Color, +8; accelerated storage stability, filtration discontinued after 2 hours due to severe plugging (Reference 38).

3. Additional data available for Paraho - SOHIO Toledo DFM: Thermal oxidation stability, JFTOT at 260°C - TDR spun, 11.5, TDR spot, 19; visual tube rating, 3. Visual appearance, white/clear; color (ASTM rating), <0.5; accelerated stability (mg/100 ml), 0.20 (Reference 67).

4. 0.5 mg/l particulate matter reported for Paraho SOHIO Toledo diesel fuel marine (Reference 67).

5. Total wax content, 0.93 wt % for Paraho - SOHIO Gary Western DFM/DF-2 (Reference 38).

6. The following relative distribution of N-PNA compound types was reported for Paraho - SOHIO Toledo DFM based on GC-MS data: (a) pyrroles, 4; (b) quinolines, 31; (c) phenyl pyridines, 16; (d) carbazoles, 48 (Reference 31).

7. A basic nitrogen value of 651 ppm was reported for Paraho - SOHIO Gary Western DFM/DF-2 (Reference 38).

8. Data are unavailable on individual oxygen-containing and sulfur-containing compounds or compound classes in petroleum and shale-derived diesel fuel.

Part V. Residual Fuel

Part V. Residual Fuel

Table 140. Specific Gravity

Material	Value	Sample Description/Source	Reference
Petroleum residual fuel	NA	--	--
Residual fuel	0.9940 (60°F)	NA	11
	0.9533 (72°F)	NA	14
Shale residual fuel			
Heavy fuel oil	0.9415	Paraho - SOHIO Gary Western	38

Table 141. API Gravity

Material	Value (°)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 fuel oil	18.5*	Average of 4 Eastern region samples	22
	21.1*	Average of 3 Central region samples	22
	19.1*	Average of 3 Rocky Mtn. region samples	22
	13.2*	Average of 3 Western region samples	22
Grade 6 fuel oil	15.7*	Average of 34 Eastern region samples	22
	13.8*	Average of 18 Southern region samples	22
	13.0*	Average of 25 Central region samples	22
	11.5*	Average of 10 Rocky Mtn. region samples	22
	13.9*	Average of 20 Western region samples	22
	25.0 (60°F)	NA	8
Shale residual fuel			
Residual fuel	29.6	Paraho - SOHIO Toledo	33
Heavy fuel oil	18.8	Paraho - SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-287

Table 142. Viscosity

Material	Value (Centistokes)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 fuel oil	148.0*	Average of 4 Eastern region samples	22
	141.6*	Average of 3 Central region samples	22
	138.1*	Average of 3 Rocky Mtn. region samples	22
	121.4*	Average of 3 Western region samples	22
Grade 6 fuel oil	160.9†	Average of 34 Eastern region samples	22
	163.5†	Average of 18 Southern region samples	22
	191.2†	Average of 25 Central region samples	22
	173.4†	Average of 10 Rocky Mtn. region samples	22
	141.9†	Average of 20 Western region samples	22
Residual fuel	300 - 700 SSU at 122°F	NA	8
	1,345 X 10- m^2/S at 82°F	NA	11
	>835 (furol seconds) at 100°F	NA	14

(Continued)

Table 142 (Concluded)

Material	Value (Centistokes)	Sample Description/Source	Reference
Shale residual fuel			
Hydrotreated residue	9.068 at 140°F[‡] (too waxy)	Paraho - SOHIO Toledo	35
Residual fuel	2.000 at 210°F	Paraho - SOHIO Toledo	33
Heavy fuel oil	142 SSU at 122°F	Paraho - SOHIO Gary Western	38

Explanatory Notes

[*] Determined via ASTM D-445 at 100°F

[†] Determined via ASTM D-88 at 122°F; units are Furol seconds rather than centistokes

[‡] Determined via ASTM D-445

Table 143. Pour Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 fuel oil	0 - 55*	Range of 4 Eastern region samples	22
	0 - 55*	Range of 3 Central region samples	22
	0 - 85*	Range of 3 Rocky Mtn. region samples	22
	-15 to 5*	Range of 3 Western region samples	22
Grade 6 fuel oil	15 - 100*	Range of 34 Eastern region samples	22
	15 - 80*	Range of 18 Southern region samples	22
	0 - 80*	Range of 25 Central region samples	22
	30 - 95*	Range of 10 Rocky Mtn. region samples	22
	-20 to 100*	Range of 20 Western region samples	22
Residual fuel	95	NA	8
	40	NA	10
	21	NA	11
	75	NA	14
FCC cycle oil	10.4	NA	57
Shale residual fuel			
Hydrotreated residue	95*	Paraho - SOHIO Toledo	35
Residual fuel	80	Paraho - SOHIO Toledo	33
Heavy fuel oil	95	Paraho - SOHIO Gary Western	38
Reduced syncrude	81	NA	57

Explanatory Notes

*Determined via ASTM D-97

Table 144. Carbon Residue

Material	Value (wt. %)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 heating oil	6.04*	Average of 4 Eastern region samples	22
	5.9*	Average of 3 Central region samples	22
	5.18*	Average of 3 Rocky Mtn. region samples	22
	8.37*	Average of 3 Western region samples	22
Grade 6 heating oil	7.78*	Average of 34 Eastern region samples	22
	8.04*	Average of 18 Southern region samples	22
	6.64*	Average of 25 Central region samples	22
	9.99*	Average of 10 Rocky Mtn. region samples	22
	10.2*	Average of 20 Western region samples	22
Shale residual fuel			
Residual fuel	0.096[†]	Paraho - SOHIO Toledo	33
Heavy fuel oil	1.50	Paraho - SOHIO Gary Western	38
	1.10[†]	Paraho - SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-524

[†] Ramsbottom carbon

Table 145. Density

Material	Value (g/ml)	Sample Description/Source	Reference
Petroleum residual fuel	NA	--	--
Shale residual fuel			
Hydrotreated residue	0.8880*	Paraho - SOHIO Toledo	35
Reduced syncrude	0.8900	NA	57

Explanatory Notes

*Determined via ASTM D-1481

Table 146. Reid Vapor Pressure

Material	Value (psi)	Sample Description/Source	Reference
Petroleum residual fuel	NA	--	--
Shale residual fuel	NA	--	--
Reduced syncrude	<0.1	NA	57

Table 147. Distillation Data

Material	Value (% evaporation)	Sample Description/Source	Reference
Petroleum residual fuel			
Residual fuel	356°F - IBP	NA	14
	482°F - 10		
	676°F - 50		
	833°F - 90		
	914°F - EP		
Shale residual fuel	331°F - IBP*	Paraho - SOHIO Toledo	33
	582°F - 10		
	732°F - 50		
	900°F - 90		
	1032°F - EP		

Explanatory Notes

*Determined via ASTM D-2887

Table 148. GC Simulated Distillation Data*

Material	Boiling Point Range (°C)	Sample Description/Source	Reference
Petroleum residual fuel	NA		
Shale residual fuel			
Hydrotreated residue	5% recovered - 256	Paraho - SOHIO Toledo	57
	50% recovered - 389		
	95% recovered - 530		
	95.4% recovered - 535		
Reduced syncrude	5% recovered - 366	NA	57
	50% recovered - 427		
	95% recovered - 529		
	96.5% recovered - 535		

Explanatory Notes

*GC simulated distillation involves use of gas chromatograph rather than distillation column. Retention times of sample peaks are based on retention times of a calibration mixture of C_3 to C_{42} normal paraffins. The boiling range distribution of the sample is calculated in weight percent via computer. Volume percent values are calculated from a density - boiling point correlation of normal paraffins (Reference 35).

Table 149. Bottom Sediment and Water

Material	Value (Vol. %)		Sample Description/Source	Reference
Petroleum residual fuel				
Grade 5 heating oil	0.12*		Average of 4 Eastern region samples	22
	0.07*		Average of 3 Central region samples	22
	0.03*		Average of 3 Rocky Mtn. region samples	22
	0.1*		Average of 3 Western region samples	22
	Water by distillation†	Sediment by extraction (wt. %)‡		
Grade 6 heating oil	0.08	0.08	Average of 34 Eastern region samples	22
	0.06	0.05	Average of 18 Southern region samples	22
	0.11	0.08	Average of 25 Central region samples	22
	0.06	0.039	Average of 10 Rocky Mtn. region samples	22
	0.13	0.04	Average of 20 Western region samples	22
Shale residual fuel				
Hydrotreated residue	0.5§		Paraho - SOHIO Toledo	35
Heavy fuel oil	0.0 (water by distillation) 0.013 (sediment by extraction)		Paraho - SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-1796

†Determined via ASTM D-95

‡Determined via ASTM D-473

§Determined via ASTM D-96

Table 150. Total Acid Number

Material	Value (mg KOH/g)	Sample Description/Source	Reference
Petroleum residual fuel	NA	--	--
Shale residual fuel	NA	--	33
Reduced syncrude	0.03	NA	57

Table 151. Flash Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 heating oil	186 - 240*	Range of 4 Eastern region samples	22
	170 - 240*	Range of 3 Central region samples	22
	136 - 236*	Range of 3 Rocky Mtn. region samples	22
	180 - 198*	Range of 3 Western region samples	22
Grade 6 heating oil	163 - 320*	Range of 34 Eastern region samples	22
	168 - >220*	Range of 18 Southern region samples	22
	184 - 348*	Range of 25 Central region samples	22
	168 - 316*	Range of 10 Rocky Mtn. region samples	22
	154 - 230*	Range of 20 Western region samples	22
	>200	NA	8
Shale residual fuel			
Heavy fuel oil	305	Paraho - SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-93

Table 151. Flash Point

Material	Value (°F)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 heating oil	186 - 240*	Range of 4 Eastern region samples	22
	170 - 240*	Range of 3 Central region samples	22
	136 - 236*	Range of 3 Rocky Mtn. region samples	22
	180 - 198*	Range of 3 Western region samples	22
Grade 6 heating oil	163 - 320*	Range of 34 Eastern region samples	22
	168 - >220*	Range of 18 Southern region samples	22
	184 - 348*	Range of 25 Central region samples	22
	168 - 316*	Range of 10 Rocky Mtn. region samples	22
	154 - 230*	Range of 20 Western region samples	22
	>200	NA	8
Shale residual fuel			
Heavy fuel oil	305	Paraho - SOHIO Gary Western	38

Explanatory Notes

*Determined via ASTM D-93

Table 152. Oxygen Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 6 fuel oil	0.19	NA	9
Shale residual fuel			
Hydrotreated residue	0.033	Paraho - SOHIO Toledo	35
Residual fuel residue	0.0182	Paraho - SOHIO Toledo	33
Reduced syncrude	0.034	NA	57

Table 153. Sulfur Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 5 fuel oil	1.02*	Average of 4 Eastern region samples	22
	0.93*	Average of 3 Central region samples	22
	1.43*	Average of 3 Rocky Mtn. region samples	22
	1.39*	Average of 3 Western region samples	22
Grade 6 fuel oil	1.41*	Average of 34 Eastern region samples	22
	1.87*	Average of 18 Southern region samples	22
	1.73*	Average of 25 Central region samples	22
	1.46*	Average of 10 Rocky Mtn. region samples	22
	1.49*	Average of 20 Western region samples	22
Residual fuel	0.24	NA	8
	0.70	NA	9
	0.49	NA	11
	0.48	NA	14
Shale residual fuel			
Hydrotreated residue	0.0005	Paraho - SOHIO Toledo	35
Residual fuel	<0.002	Paraho - SOHIO Toledo	33
Heavy fuel oil	0.25	Paraho - Gary Western	38
Reduced syncrude	0.0025	NA	57

Explanatory Note

*Determined via ASTM D-129

Table 154. Nitrogen Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 6 fuel oil	0.23	NA	8
	0.30	NA	9
Residual fuel	0.27	NA	10
	0.23	NA	11
	0.22	NA	14
Shale residual fuel			
Hydrotreated residue	0.046	Paraho - SOHIO Toledo	35
Residual fuel	0.44	Paraho - SOHIO Toledo	33
Heavy fuel oil	1.73	Paraho - Gary Western	38
Reduced syncrude	0.0150	NA	57

Table 155. Carbon Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 6 fuel oil	87.02	NA	8
	87.0	NA	9
Residual fuel	87.39	NA	10
Shale residual fuel			
Hydrotreated residue	87.1	Paraho - SOHIO Toledo	35
Residual fuel	86.71	Paraho - SOHIO Toledo	33

Table 156. Hydrogen Content

Material	Value (Wt. %)	Sample Description/Source	Reference
Petroleum residual fuel			
Grade 6 fuel oil	12.49	NA	8
	11.0	NA	9
Residual fuel	11.24	NA	10
	11.52	NA	11
	11.43	NA	14
Shale residual fuel			
Hydrotreated residue	12.9	Paraho - SOHIO Toledo	35
Residual fuel	12.75	Paraho - SOHIO Toledo	33

Table 157. Trace Elements Content (ppmw)*

Material	Al	Sb	As	Be	Cd	Ca	Cl	Co	Cr	Cu
Petroleum residual fuel										
Residual oil	NA	NA	0.51	0.10	0.30	NA	NA	NA	0.90	NA
FCC cycle oil	NA	<0.5	<0.3	NA	<0.03	NA	NA	NA	<0.05	<0.05
Shale residual fuel										
Hydrotreated residue	0.055 (FE)	ND(<3) (XRF)	ND(<0.5) (XRF)	<0.005 (AA)	<0.005 (AA)	0.26 (FE)	ND(<2) (XRF)	<0.03 (FE)	0.010 (FE)	0.023 (AA)
Residual fuel	NA	NA	<0.4	NA	NA	NA	NA	NA	NA	NA
Reduced syncrude	NA	ND(<0.5)	0.9	NA	ND(<0.03)	NA	NA	NA	0.05	0.07

Material	Fe	Pb	Mg	Mn	Hg	Mo	Ni	Se	Si	Ag	Na
Petroleum residual fuel											
Residual oil	NA	NA	NA	0.57	0.066	0.52	19	1.1	NA	NA	NA
FCC cycle oil	<0.05	<0.06	NA	NA	<1	NA	<0.05	<0.3	NA	NA	NA
Shale residual fuel											
Hydrotreated residue	0.41 (FE)	<0.05 (FE)	0.052 (AA)	0.004 (FE)	ND(<2) (XRF)	<0.02 (FE)	<0.05 (FE)	ND(<0.5)	0.35 (AA)	<0.01 (FE)	0.11 (FE)
Residual fuel	0.10	NA	NA	NA	NA	NA	NA	NA	NA	NA	<0.6
Reduced syncrude	0.3	0.2	NA	NA	3†	NA	ND(<0.05)	ND<0.3	NA	NA	NA

(Continued)

Table 157 (Concluded)

Material	Sr	Th	Sn	Ti	V‡	Zn	Sample Description/Source	Reference
Petroleum residual fuel								
Residual oil	NA	NA	NA	NA	31	NA	Average of 11 residual oils	24
FCC cycle oil	NA	NA	NA	NA	<0.05	0.1	NA	57
Shale residual fuel								
Hydrotreated residue	0.004 (FE)	ND(<6)	<0.5 (AA)	ND(<0.4) (XRF)	<0.03 (FE)	0.28 (AA)	Paraho - SOHIO Toledo	35
Residual fuel	NA	NA	NA	NA	<0.02	NA	Paraho - SOHIO Toledo	33
Reduced syncrude	NA	NA	NA	NA	0.07	0.1	NA	57

Explanatory Notes

*Methods used include atomic absorption spectroscopy (AA), flame emission spectroscopy (FE), neutron activation analysis (NAA), and X-ray fluorescence (XRF).

†Result may be an artifact of laboratory processing, since no mercury was detected in the raw shale oil.

‡26 ppmw vanadium has also been reported for a petroleum-derived residual oil (Reference 11).

Table 158. Saturates, Olefins and Aromatics Contents

Material	Value	Sample Description/Source	Reference
Petroleum residual fuel	NA*	--	--
Shale residual fuel			
Residual fuel		Paraho - SOHIO Toledo	33
Saturates	64.1		
Olefins	0.00		
Aromatics	35.9		
Heavy fuel oil		Paraho - SOHIO Gary Western	38
Saturates	26.2		
Olefins	19.7		
Aromatics	54.1		

Explanatory Notes

*A benzene content of 4 ppmw is reported for a fluid catalytic cracker (FCC) cycle oil in Reference 57; a description of sample source is not provided.

Table 159. Detailed Hydrocarbon Class Analysis

	Value*			
Material	Compound Class	Vol %	Sample Description/Source	Reference
Petroleum residual fuel	NA	NA	--	--
Shale residual fuel Hydrotreated residue	IBP-400°F Cut		Paraho - SOHIO Toledo	35
	n-Paraffins	30.7		
	iso-paraffins	8.7		
	Total Paraffins	39.4		
	Cyclopentanes	12.1		
	Cyclohexanes	22.1		
	Total Monocycloparaffins	34.2		
	Total Dicycloparaffins	6.4		
	Total Saturates	80.0		
	Benzene	0.1		
	Toluene	0.3		
	C_8 Aromatics	3.5		
	C_9 Aromatics	5.8		
	C_{10} Aromatics	3.3		
	C_{11} Aromatics	1.4		
	C_{12} Aromatics	0.6		
	Total Alkylbenzenes	15.0		
	Total Indans + tetralins	4.7		

(Continued)

Table 159 (Continued)

Material	Value*		Sample Description/Source	Reference
	Compound Class	Wt %		
Shale residual fuel Hydrotreated residue			Paraho - SOHIO Toledo	35
	C10 Naphthalenes	0.1		
	C11 Naphthalenes	0.1		
	C12 Naphthalenes	0.1		
	Total Naphthalenes	0.3		
	Total Aromatics	20.0		
	400-650°F Cut			
	Paraffins	34.1		
	Mononaphthenes	16.2		
	Polynaphthenes	12.9		
	Total Saturates	63.2		
	Alkylbenzenes	7.1		
	Indans + tetralins	10.2		
	Dinaphthenebenzenes	6.2		
	Total Monoaromatics	23.5		
	Naphthalenes	1.6		
	Biphenyls	2.9		
	Fluorenes	2.0		
	Total diaromatics	6.5		
	Phenanthrenes	2.2		
	Naphphenanthrenes	0.6		
	Total Triaromatics	2.8		
	650-850°F Cut			
	Paraffins	30.8		
	Monoaphthenes	12.4		
	Polynaphthenes	11.8		
	Total Saturates	55.0		

(Continued)

Table 159 (Concluded)

	Value*			
Material	Compound Class	Wt %	Sample Description/Source	Reference
Shale residual fuel Hydrotreated residue	650-850°F Cut		Paraho - SOHIO Toledo	35
	Alkylbenzenes	5.3		
	Indans + tetralins	11.5		
	Dinaphthenebenzenes	7.9		
	Total monoaromatics	24.7		
	Biphenyls	4.3		
	Fluorenes	2.3		
	Total diaromatics	6.6		
	Phenanthrenes	4.0		
	Naphphenanthrenes	0.9		
	Total triaromatics	4.9		
	Pyrenes	0.7		
	Total Tetraaromatics	0.7		
	Total Pentaaromatics	1.5		
	Total Aromatics	38.4		
	850°F+ Cut			
	Saturates	55.5		
	Aromatics†	35.0		
	Asphaltics†	1.6		

Explanatory Notes

*Determined by mass spectrometry and liquid chromatography.

†Sulfur-containing compounds are included in these groups.

Table 159 (Concluded)

Material	Value[*]		Sample Description/Source	Reference
	Compound Class	Wt %		
Shale residual fuel Hydrotreated residue	650-850°F Cut		Paraho - SOHIO Toledo	35
	Alkylbenzenes	5.3		
	Indans + tetralins	11.5		
	Dinaphthenebenzenes	7.9		
	Total monoaromatics	24.7		
	Biphenyls	4.3		
	Fluorenes	2.3		
	Total diaromatics	6.6		
	Phenanthrenes	4.0		
	Naphphenanthrenes	0.9		
	Total triaromatics	4.9		
	Pyrenes	0.7		
	Total Tetraaromatics	0.7		
	Total Pentaaromatics	1.5		
	Total Aromatics	38.4		
	850°F+ Cut			
	Saturates	55.5		
	Aromatics[†]	35.0		
	Asphaltics[†]	1.6		

Explanatory Notes

[*] Determined by mass spectrometry and liquid chromatography.

[†] Sulfur-containing compounds are included in these groups.

Table 160. Detailed PNA Composition

Material	Value*		Sample Description/Source	Reference
	Compound	µg/g		
Petroleum residual fuel	NA	NA	--	--
Shale residual fuel				
Hydrotreated residue	Fluorene	14	Paraho - SOHIO Toledo	31
	Phenanthrene	124		
	Anthracene	<10		
	Fluoranthene	109		
	Pyrene	287		
	Benz(a)anthracene	10		
	Chrysene	16		
	Triphenylene	1.7		
	Me-B(a)A	58		
	DMe/Et-B(a)A	48		
	Benzo(g,h,i)fluoranthene	276		
	Benzo(b)fluoranthene	<12		
	Benzo(j)fluoranthene	<11		
	Benzo(k)fluoranthene	1.6		
	Perylene	3.7		
	Benzo(e)pyrene	54		
	Benzo(a)pyrene	14		
	Methyl B(e)P	39		
	Methyl B(a)P	11		
	1,2,3 Indeno (c,d)pyrene	< 1.1		
	Dibenz(a,h)anthracene	< 3.9		
	Benzo(g,h,i)perylene	83		
	Coronene	11		

Explanatory Notes

*Determined by GC/UV methods

Table 161. Nitrogen Compound Class Analysis - Solvent Fractionation ("Type 1")*

A. Compound Type Fractions and Elemental Nitrogen Content of Fractions

Material	Nitrogen, wt. % of Fraction Hydrocarbon	Pyridine I	Pyrrole	Pyrrole/Arylamine	Pyridine II	Amide/Pyridine III	Sample Description/Source	Reference
Petroleum residual fuel	NA	NA	NA	NA	NA	NA	--	--
Shale residual fuel								
Hydrotreated residue[†]	0.004	3.48	1.74	5.86	4.17	3.91	Paraho - SOHIO Toledo	53

B. Potentiometric Titration Results for Compound Type Fractions

Material	Nitrogen Type Fractions	Nitrogen, wt. % of Fraction Strong Base pKa 9 to 11	Weak Base I, pKa 7 to 9	Weak Base II, pKa 2 to 7	Weak Base II, pKa 2 to 7	Very Weak Base pKa-2 to 2	Nonbasic Nitrogen Compounds	Total	Sample Description/Source	Reference
Petroleum residual fuel	--	NA	NA	NA	NA	NA	NA	NA	--	--
Shale residual fuel										
Hydrotreated residue	Pyridine I	ND	3.36	ND	ND	ND	0.12	3.48	Paraho - SOHIO Toledo	53
	Pyrrole	ND	ND	0.11	ND	0.64	0.99	1.74		
	Pyrrole/Arylamine	ND	ND	0.02	0.16	2.02	3.66	5.86		
	Pyridine II	ND	3.92	ND	ND	ND	0.25	4.17		
	Amide/Pyridine II	ND	1.59	0.75	ND	0.88	0.69	3.91		

(Continued)

Table 161 (Concluded)

C. Nitrogen - Compound Type Fraction Distribution

Nitrogen Compound Type	Nitrogen, wt. % of Sample Petroleum Residual Fuel	 Shale Residual Paraho - SOHIO Toledo DFM (Ref. 53)
Strong Base	NA	
Alkylamines/alkylpiperidines		ND
Weak base I	NA	
Hindered alkylpyridines/alkylquinolines		0.090
Less hindered alkylpyridines/alkyliquinolines/alkylacridines		0.165
Less hindered alkylpyridines/alkylquinolines/alkylhydropyridines		0.008
Weak base II	NA	
Alkylnaphthenopiperidines		0.004
Unknown		0.001
Weak base II	NA	
Alkylanilines/alkylnaphthenoanilines		0.003
Very weak base	NA	
Alkylhydroxypyridines		0.004
Alkylpyrroles/alkylindoles		0.043
Unknown		--
Nonbasic	NA	
N-Alkylcarbazoles		0.003
Alkylpyrroles/alkylindoles/alkylcarbazoles/alkylbenzocarbazoles		0.078
Alkylcarboxamides/alkyldiazaaromatics		0.014
Total	NA	0.413

Explanatory Notes

*This solvent fractionation method involves separation of the sample into six compound-type fractions using basic/neutral alumina and silica adsorption chromatography; method is described in References 32 and 53.

†Original sample contained 0.42 wt. % of nitrogen; the cumulative nitrogen in the fractions is 0.412 wt. %, or 98% of the original sample.

Table 162. Detailed N-PNA Composition

Material	Value*,†			Sample Description/Source	Reference
	Z No.	Compound	Relative Distribution		
Petroleum residual fuel	NA	NA	NA	--	--
Shale residual fuel					
Hydrotreated residue	3	Pyrroles	1	Paraho - SOHIO Toledo	31
	5	Pyridines	15		
	7	Azaindanes	9		
	9	Indoles	5		
	11	Quinolines	8		
	13	Phenyl pyridines	7		
	15	Carbazoles	14		
	17	Acridines	14		
	19	Benzo(d,e,f)carbazoles	4		
	21	Azapyrenes, Benzcarbazoles	13		
	23	Benzacridines	4		
	27	Dibenzcarbazoles	1		
	29	Dibenzacridines	0.2		

Explanatory Notes

*Determined by mass spectrometry.

†Only nitrogen-containing masses were determined in the samples; all data are normalized to 100% (wt/wt) in order to determine relative compound distribution (see also Table 40).

GENERAL COMMENTS

1. Additional data for Paraho - SOHIO Toledo hydrotreated residue: cryoscopic molecular weight, 300 (Reference 35).

2. Additional data for Paraho - SOHIO Gary Western heavy fuel oil: fire point, 435°F; gross heat of combustion, 18,003 Btu/lb; net heat of combustion, 17,263 Btu/lb; corrosion, 1A at 3 hr/212°F; aniline point, 129.6°F; thermal stability - No. 1, stable; explosiveness, 5% (Reference 38).

3. Additional data for petroleum-derived Grade 6 fuel oil: heating value, 19,200 Btu/lb (Reference 83); 18,610 Btu/lb (Reference 9).

4. Additional data for petroleum residual fuel: net heat of combustion, 17,768 Btu/lb (Reference 11); 17,609 Btu/lb (Reference 14).

5. Elemental composition of petroleum-derived blown asphalt: 85.2% carbon, 7.4% hydrogen, 6.7% oxygen and 0.7% sulfur (Reference 74).

6. Available data for API petroleum coke (range of six samples, wt. %): carbon, 82.85-90.17; hydrogen, 2.15-11.94; oxygen, 0.89-3.75; sulfur, 1.97-6.08; nitrogen, 0.14-1.45. Additional data for 3 samples: free silica content (ppm), 24-98; wt. % SiO_2, 0.04; wt. % Fe_2O_3, 0.06-1.13; wt. % ash, 0.21-0.81; trace metals - <1 ppb As, 0.7-5.3 ppm Se, <1-113,100 ppb Hg, 120-410 ppm V, 60-160 ppm Ni (Reference 71).

7. A value of 5.23 wt. % wax has been reported for Paraho - SOHIO Gary Western heavy fuel oil (Reference 38).

8. Additional PNA data for four API petroleum coke samples (detection limit, 1 ppm) (Reference 71):

PNA	Value, ppm			
	1	2	3	4
Benzo(a)pyrene	10	440	50	1,680
Benzo(e)pyrene	4	110	197	27
Benzo(g,h,i)perylene	9	439	276	187
Benzo(a)anthracene	4	544	38	108
Dibenzo(a,h)anthracene	4	ND	35	ND
Chrysene	2	126	138	ND
Pyrene	8	ND	314	ND
Benzo(b)fluoranthene	ND	ND	176	ND
Phenanthrene	ND	ND	280	ND
Methyl Benzo(a)pyrene	ND	ND	32	ND
Fluorene	ND	11	ND	ND
Benzo(g,h,i)fluoranthene	ND	ND	ND	ND
Benzofluorenes	ND	ND	ND	ND
Perylene	ND	ND	ND	ND
Coronene	ND	ND	ND	ND

9. Molecular parameter data calculated using 1H/13CNMR data on 3 petroleum-derived residuals: (a) petroleum pitch; (b) decant oil from a catalytic cracking operation; and (c) an ethylene tar residue from distillation of the residual product from an ethylene plant (Reference 73):

Parameter	Petroleum pitch	Decant oil residue	Ethylene tar residue
η	1.8	2.6	1.6
fc	5.1	5.8	6.2
x	2.4	2.1	1.9
No. C_A	29.1	12.5	28.7
No. C_1	17.1	9.0	20.7
R_A	7.1	2.8	5.0
AS	22.7	30.0	25.5
R_S	3.9	2.7	5.3
R_N	0.8	1.1	2.9
No. C_{AI}	6.9	7.0	8.6
No. H_{AI}	16.2	14.6	16.7

Equations used for calculation of molecular parameters presented on previous page.

Symbol	Average parameter	Equation
n	Carbons per alkyl side chain	$\frac{H_\alpha + H_\beta + H_\gamma}{H}$
f_c	Carbon-hydrogen weight ratio of total alkyl groups	$\frac{C\ C_{AI}}{H\ H_{AI}}$
x	Hydrogen-carbon atomic ratio of alkyl groups	$12/f_c$
C_A	Percent aromatic carbon	$C\ C_{Ar}$
C_1^s	Percent substituted aromatic carbon	$\frac{C\ C_{AI}}{n}$
C_1^u	Percent unsubstituted aromatic carbon	$12\ H_{Ar}\ H$
C_1	Percent nonbridge aromatic Carbon	$C_1^s + C_1^u$
No. C_A	Aromatic carbons per average molecule	$\frac{C_A\ M}{1200}$
No. C_1	Aromatic nonbridge carbons per average molecule	$\frac{C_1\ M}{1200}$
R_A	Aromatic rings per average molecule	$\frac{\text{No. } C_A - \text{No. } C_1}{2} + 1$
AS	Percent substitution of aromatic rings	$\frac{100\ C_1^s}{C_1}$
R_S	Alkyl substituents per average molecule	$\frac{\text{AS No. } C_1}{100}$
R_N	Napthenic rings per average molecule	$RS\ (n + 0.5) - \frac{6n}{f_c}$
No. C_{AI}	Aliphatic carbons per average molecule	$n\ R_S$
No. H_{AI}	Aliphatic hydrogens per average molecule	$n \times R_S$